Supporting information for:

Role of intramolecular hydrogen bonds in promoting electron flow through amino-acid and oligopeptide conjugates

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Table of Contents

1. Synthetic procedures

All the reactions were carried out in flame-dried glassware in argon atmosphere. Required chemicals were purchased from Sigma-Aldrich and used without further purification. Fmoc-protected tetra-*L*-alanine was bought from ChinaPeptides and used as received. DMF was dried using solvent purification system. The reaction progress was monitored by thin layer chromatography (TLC, aluminum plates coated with silica gel, Merck 60, F-254) and visualized via UV lamp. The ^{1}H, ^{13}C NMR spectra were measured at temperature 298 K in $CDCl_3$ (if not otherwise stated) solutions with a Varian vnmrs-600, using tetramethylsilane (TMS) as internal standard. The structures of the compounds studied were confirmed by 2D NMR spectra: COSY, $^{1}H–^{13}C$ HSQC, $^{1}H–^{13}C$ HMBC, ROESY. Due to the compound dynamics values given with the "u" appendix are averaged from two signals. Perylene bisimide derivatives **1**, **15** and corrole **8** were synthesized according to the reported procedures. [1, 2]

General procedure for compounds **5**-**7**: Perylene **1** (101 mg, 0.192 mmol), HATU (73 mg, 0.192 mmol), DIPEA (50 µl, 0.288 mmol) were dissolved in dry DMF (18 mL) and stirred for 30 minutes under argon atmosphere. Subsequently corresponding amino-acid (0.192 mmol) was added and the resulting solution was stirred for 2h. After concentration *in vacuo* the purification of each compound is described as follows.

Compound **5**: Following the general procedure perylene **1** was reacted with aminoacid **2**. The crude reaction mixture was purified by column chromatography (silica, 2% MeOH:DCM) and crystalized from diethyl ether giving red crystals of **5** (77% yield).

^{1}H NMR (600 MHz, $CDCl_3$) δ (ppm): 8.58 – 8.47 (bs, 2H), 8.40 (d, *J* = 7.8 Hz, 2H), 8.34 (d, *J* = 8.0 Hz, 2H), 8.27 (d, *J* = 8.0 Hz, 2H), 7.67 – 7.62 (m, 2H), 7.57 (d, *J* = 7.5 Hz, 2H), 7.35 – 7.22 (m, 4H), 7.01 – 6.96 (bs, 1H), 5.61 (bs, 1H), 5.20 – 5.12 (m, 1H), 4.45 – 4.27 (m, 3H), 4.25 – 4.12 (m, 3H), 3.38 – 3.30 (m, 2H), 2.29 – 2.19 (m, 2H), 2.03 – 1.96 (m, 2H), 1.93 – 1.84 (m, 2H), 1.49 (d, *J* = 7.0 Hz, 3H), 1.40 – 1.18 (m, 16H), 0.82 (t, *J* = 6.9 Hz, 6H);

^{13}C NMR (150 MHz, $CDCl_3$) δ (ppm): 172.3, 163.8u, 163.5, 155.9, 143.8u, 141.2, 134.6, 133.7, 131.3, 131.2u, 129.3, 129.1, 127.6, 127.0, 126.0, 125.9, 125.1, 123.7u, 123.0, 122.7, 122.5, 119.9, 67.1, 54.9, 50.8, 47.1, 37.7, 36.4, 32.4, 31.8, 29.2, 27.8, 27.0, 22.6, 19.0, 14.0;

TOF MS ES-. Mass 945.4203. Calculated for C58, H58, N4, O7, Na: 945.4203.

Compound **6**: Following the general procedure perylene **1** was reacted with aminoacid **3**. The crude reaction mixture was purified by column chromatography (silica, 5% MeOH:DCM) and crystalized from diethyl ether giving red crystals of **6** (53% yield).

^{1}H NMR (600 MHz, DMF-d6) δ (ppm): 8.81 – 8.77 (m, 2H), 8.74 - 8.71 (m, 2H), 8.56 – 8.47 (m, 2H), 8.43 – 8.38 (m, 2H), 8.29 (d, *J* = 6.7 Hz, 1H), 8.11 (d, *J* = 8.5 Hz, 1H), 8.04 – 7.99 (m, 1H), 7.92 – 7.87 (m, 1H), 7.80 -7.75 (m, 2H), 7.70 – 7.63 (m, 3H), 7.36 – 7.22 (m, 4H), 5.24 – 5.15 (m, 1H), 4.41 – 4.13 (m, 9H), 3.37 – 3.27 (m, 2H), 2.38 – 2.30 (m, 2H), 2.00 – 1.85 (m, 4H), 1.45 – 1.17 (m, 28H), 0.82 (t, *J* = 6.9 Hz, 6H);
^{13}C NMR (150 MHz, DMF-d6) selected signals δ (ppm): 173.6, 172.9, 172.6, 172.4, 164.2u, 163.4, 156.8, 144.4, 141.3, 134.6, 131.4u, 131.2, 128.0, 127.4, 125.7, 124.3, 124.3, 120.3, 66.7, 54.3, 51.4, 49.6, 49.6, 49.6, 47.4, 38.5, 37.4, 32.6, 32.0, 29.5, 28.6, 27.2, 22.8, 18.1, 18.0, 17.6, 17.5, 13.9;

TOF MS ES+. Mass 1158.5310. Calculated for C67, H73, N7, O10, Na: 1158.5317.

Compound **7**: Following the general procedure perylene **1** was reacted with aminoacid **4**.The crude reaction mixture was purified by column chromatography (silica, 1% MeOH:DCM) and crystalized from diethyl ether giving red crystals of **7** (70% yield).

^{1}H NMR (600 MHz, $CDCl_3$) δ (ppm): 8.67 – 8.56 (bs, 2H), 8.54 - 8.48 (m, 4H), 8.45 (d, *J* = 8.1 Hz, 2H), 7.69 (d, *J* = 7.7 Hz, 2H), 7.58 – 7.52 (m, 2H), 7.39 -7.26 (m, 8H), 7.24 – 7.20 (m, 1H), 6.76 – 6.70 (bs, 1H), 5.56 – 5.47 (bs, 1H), 5.21 – 5.13 (m, 1H), 4.53 – 4.45 (m, 1H), 4.40 – 4.32 (m, 2H), 4.19 (dd, *J* = 7.2, 7.2 Hz, 1H), 4.06 – 3.98 (m, 1H), 3.96 – 3.85 (m, 1H), 3.35 – 3.04 (m, 4H), 2.28 – 2.19 (m, 2H), 1.93 – 1.75 (m, 4H), 1.40 – 1.16 (m, 16H), 0.82 (t, *J* = 6.9 Hz, 6H);
^{13}C NMR (150 MHz, $CDCl_3$) δ (ppm): 170.5, 163.9u, 163.7, 163.5, 155.9, 143.8u, 141.2u, 136.6, 134.9, 134.1, 131.6, 131.4u, 129.4, 128.7, 127.7, 127.1, 127.0, 126.3, 126.2, 125.1u, 124.1, 123.4, 123.2, 122.9, 122.6, 119.9, 67.1, 56.6, 54.8, 47.1, 39.0, 37.5, 36.1, 32.4, 31.7, 29.2, 27.8, 26.9, 22.6, 14.0.

TOF MS ES+. Mass 1021.4516. Calculated for C64, H62, N4, O7, Na: 1021.4516.

General deprotection procedure: Corresponding compounds **5**-**7** (0.100 mmol) were dissolved in 2 ml of 20% piperidine in DMF solution and stirred for 30 minutes. Each reaction mixture was concentrated *in vacuo* and used without further purification due to the limited stability.

Compound **8**: Following the general procedure crude product was washed diethyl ether giving **8** as red solid.

TOF MS ES+. Mass 701,3700. Calculated for C43, H49, N4, O5: 701,3703.

Compound **9**: Following the general procedure crude product was washed diethyl ether giving **9** as red solid.

TOF MS ES+. Mass 914,4824. Calculated for C52, H64, N7, O8: 914,4816.

Compound **10**: Following the general procedure crude product was washed diethyl ether giving **10** as red solid.

TOF MS ES+. Mass 777,4006. Calculated for C49, H53, N4, O5: 777,4016.

General procedure for corrole-perylene conjugates **12**-**14**. Corrole **11** (50 mg, 0.064 mmol), HATU (24 mg, 0.064 mmol), DIPEA (17 µl, 0.096 mmol) were dissolved in dry DMF (18 mL) and stirred for 30 minutes under argon atmosphere. Subsequently corresponding perylene derivative (0.064 mmol) was added and the resulting solution was stirred for 2h. After concentration *in vacuo* the purification of each compound is described as follows.

Cor-Ala-PDI: Following the general procedure corrole **11** was reacted with perylene-aminoacid conjugate **8**. The crude reaction mixture was purified by column chromatography (silica DCVC, ethyl acetate) and crystalized from diethyl ether giving dark red crystals of **Cor-Ala-PDI** (2 steps, 48% yield).

^{1}H NMR (600 MHz, $CDCl_3$) δ (ppm): 8.97 – 8.90 (bs, 2H), 8.68 - 8.55 (m, 4H), 8.55 – 8.47 (m, 6H), 8.42 – 8.35 (m, 4H), 8.29 – 8.24 (bs, 1H), 7.79 – 7.85 (m, 1H), 7.54 -7.48 (m, 1H), 7.18 – 7.14 (m, 1H), 5.31 – 5.25 (bs, 1H), 5.21 – 5.13 (m, 1H), 4.29 (d, *J* = 14.4 Hz, 1H), 4.14 (d, *J* = 14.4 Hz, 1H), 4.09 – 4.00 (bs, 1H), 3.42 – 3.33 (m, 1H), 3.30 – 3.22 (m, 1H), 3.01 – 2.93 (m, 1H), 2.29 – 2.15 (m, 2H), 1.91 – 1.88 (m, 2H), 1.38 – 1.14 (m, 16H), 0.81 (t, *J* = 6.9 Hz, 6H), 0.66 – 0.48 (bs, 2H), 0.43 – 0.11 (m, 2H), -0.50 - -0.85 (bs, 3H);
^{13}C NMR (125 MHz, $CDCl_3$) δ (ppm): 168.5, 166.2, 164.5, 163.4, 157.5, 147.1u, 144.9, 138.8, 136.8, 135.0, 134.0, 131.5, 131.4u, 130.9, 130.1, 129.5, 129.1, 126.3, 126.2, 123.5, 123.3, 122.8, 122.3, 121.4, 116.1, 114.3, 112.7, 107.6, 67.6, 46.0, 36.5, 33.9, 32.4, 31.7, 29.7, 29.2, 26.9, 25.6, 22.6, 17.2, 14.0;

TOF MS ES-. Mass 1461.4538. Calculated for C82, H64, N8, O7, F10: 1461.4538.

Cor-(Ala)$_4$-PDI: Following the general procedure corrole **11** was reacted with perylene-aminoacid conjugate **9**. The crude reaction mixture was purified by column chromatography (silica DCVC, 2% methanol:ethyl acetate) and crystalized from diethyl ether giving dark red crystals of **Cor-(Ala)$_4$-PDI** (2 steps, 32%).

^{1}H NMR (600 MHz, $CDCl_3$) δ (ppm): 9.21 – 8.92 (m, 2H), 8.67 - 8.10 (m, 15H), 7.78 – 7.68 (m, 1H), 7.54 – 7.44 (m, 1H), 7.36 – 7.09 (m, 2H), 6.95 – 6.75 (m, 1H), 5.99 – 5.77 (m, 1H), 5.71 – 5.46 (m, 1H), 5.20 – 5.07 (m, 1H), 4.50 – 4.01 (m, 6H), 4.00 – 3.82 (m, 1H), 3.43 – 3.07 (m, 2H), 3.03 – 2.87 (m, 1H), 2.30 – 1.78 (m, 6H), 1.39 – 0.99 (m, 22H), 0.81 (t, *J* = 6.9 Hz, 6H), -0.33 - -0.89 (m, 4H), -0.96 - -1.37 (m, 3H);
^{13}C NMR (150 MHz, $CDCl_3$) selected signals δ (ppm): (171.8, 169.7, 163.7, 157.5, 146.9, 145.1, 136.9 z C13 NMR), 134.1u, 131.5, 131.3, 130.8, 130.2, 126.5, 125.1, 122.9, 122.7, 121.4, 112.5, 67.3, 54.8, 49.3, 48.6, 46.5, 45.6, 37.6, 36.3, 32.4, 31.8, 29.2, 27.8, 26.9, 22.6, 19.5, 17.8, 17.8, 17.2, 14.0;

TOF MS ES+. Mass 1698.5737. Calculated for C91, H79, N11, O10, F10, Na: 1698.5749.

Cor-Phe-PDI: Following the general procedure corrole **11** was reacted with perylene-aminoacid conjugate **10**.The crude reaction mixture was purified by column chromatography (silica DCVC, 50% ethyl acetate:Hexane) and crystalized from diethyl ether giving dark red crystals of **Cor-Phe-PDI** (2 steps, 45%).

^{1}H NMR (600 MHz, $CDCl_3$) δ (ppm): 9.20 – 9.13 (bs, 1H), 8.95 – 8.88 (bs, 1H), 8.70 - 8.45 (m, 7H), 8.40 – 8.17 (m, 8H), 7.79 – 7.73 (m, 1H), 7.55 -7.48 (m, 1H), 7.16 – 7.10 (m, 1H), 6.84 – 6.72 (m, 3H), 5.39 – 5.21 (bs, 2H), 5.21 – 5.13 (m, 1H), 4.97 – 4.90 (m, 1H), 4.28 (d, *J* = 14.4 Hz, 1H), 4.12 (d, *J* = 14.4 Hz, 1H), 3.98 – 3.86 (bs, 1H), 3.07 – 2.95 (m, 2H), 2.29 – 2.19 (m, 2H), 2.16 – 2.06 (m, 1H), 1.93 – 1.82 (m, 2H), 1.67 – 1.58 (bs, 1H), 1.49 – 1.40 (bs, 1H), 1.39 – 1.16 (m, 16H), 0.82 (t, *J* = 6.9 Hz, 6H), 0.68 – 0.52 (bs, 1H), 0.45 – 0.13 (m, 2H), -0.45 - -0.58 (bs, 1H);
^{13}C NMR (125 MHz, $CDCl_3$) δ (ppm): 166.4, 165.9, 163.9u, 163.3, 157.4, 146.9u, 145.2u, 142.3, 140.7, 138.6, 136.9, 135.1, 134.6, 133.8, 131.5u, 131.2, 130.8u, 130.1, 129.3, 128,8, 128.2, 127.9, 126.1, 125.9, 123.7u, 123.1, 122.5, 122.0, 121.3, 116.2, 116.0, 114.4u, 112.3, 107.5, 67.2, 54.8, 52.3, 36.1, 33.6, 32.4, 31.7, 29.7, 29.2, 26.9, 25.6, 22.6, 14.0;

TOF MS ES+. Mass 1539.5142. Calculated for C88, H69, N8, O7, F10: 1539.5130.

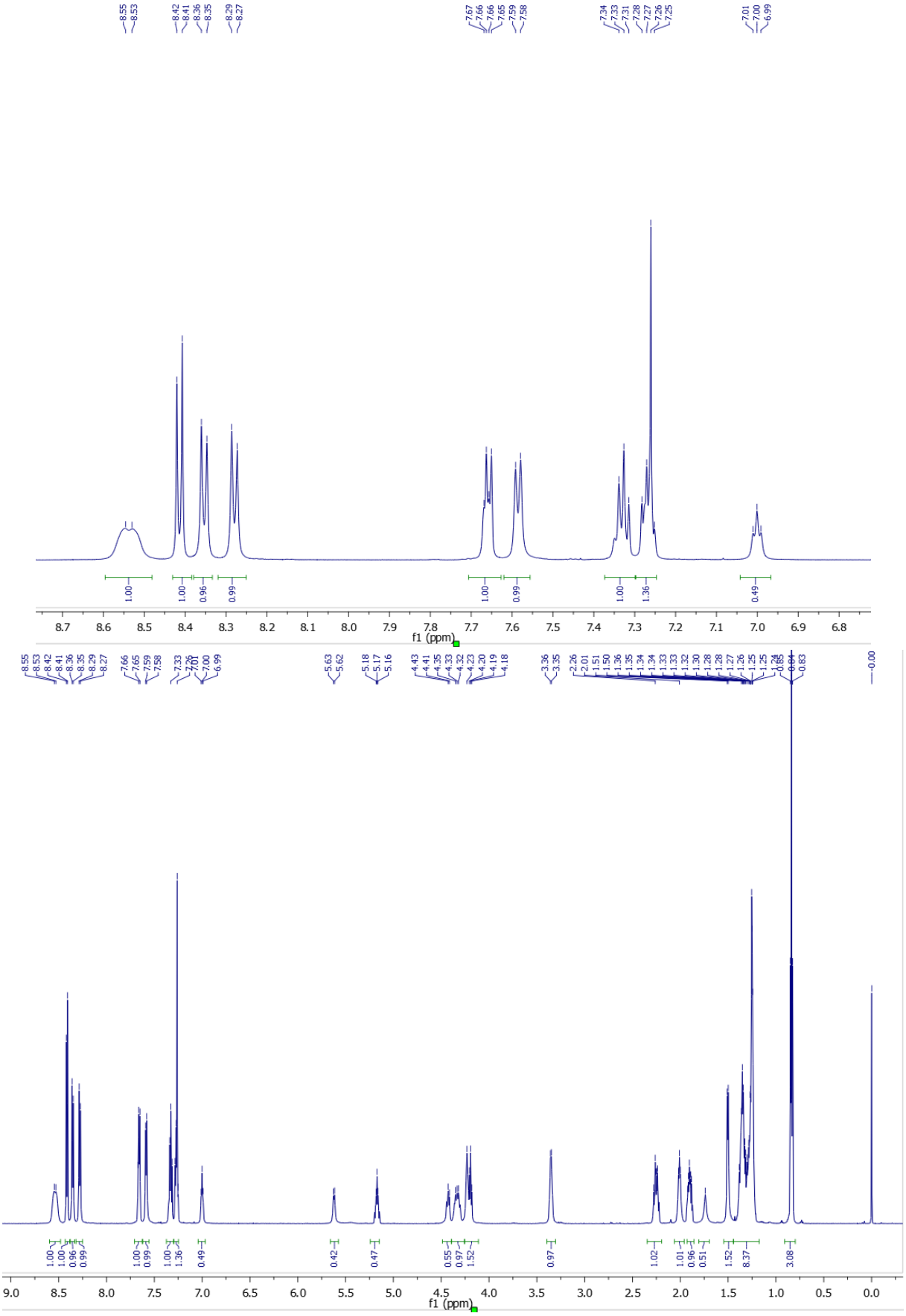
Cor-Phe: Following the general procedure corrole **11** was reacted with *L*-Phenylalanine Methyl Ester. The crude reaction mixture was purified by column chromatography (silica, 1% methanol:DCM) and crystalized from diethyl ether giving dark red crystals of **Cor-Phe** (62% yield).

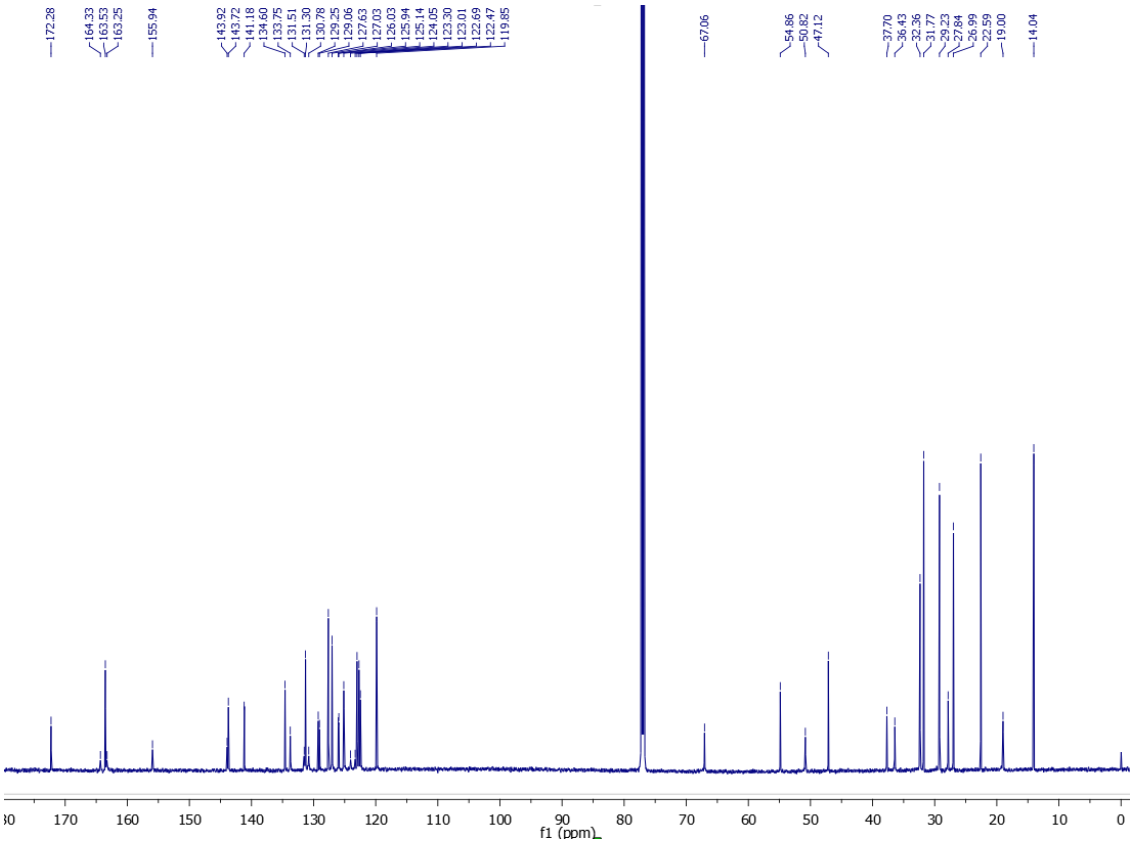
^{1}H NMR (600 MHz, DMF-d_6) δ (ppm): 9.36 – 9.17 (m, 2H), 9.13 – 8.54 (m, 4H), 8.72 – 8.53 (m, 2H), 8.14 – 8.07 (m, 1H), 7.85 – 7.76 (m, 1H), 7.52 – 7.45 (m, 1H), 7.44 – 7.37 (m, 1H), 6.72 – 6.04 (m, 4H), 5.99 – 5.57 (m, 2H), 4.58 – 4.36 (m, 2H), 4.06 – 3.96 (m, 1H), 3.29 – 3.03 (bs, 3H), 2.17 – 1.97 (m, 1H), 1.90 – 1.32 (m, 1H).

TOF MS ES-. Mass 940,1959. Calculated for C49, H28, N5, O4, F10: 940.1982.

2. NMR spectra

Compound **5**

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129.06
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19.00
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170
160
150
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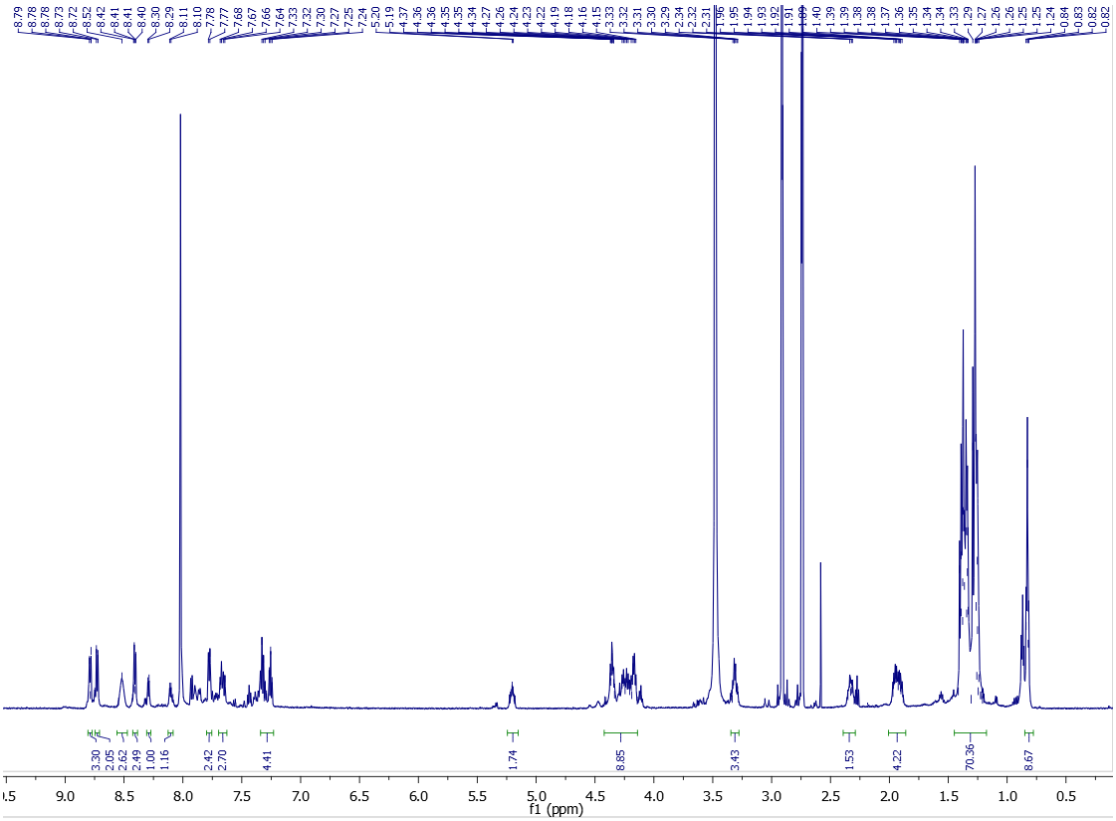
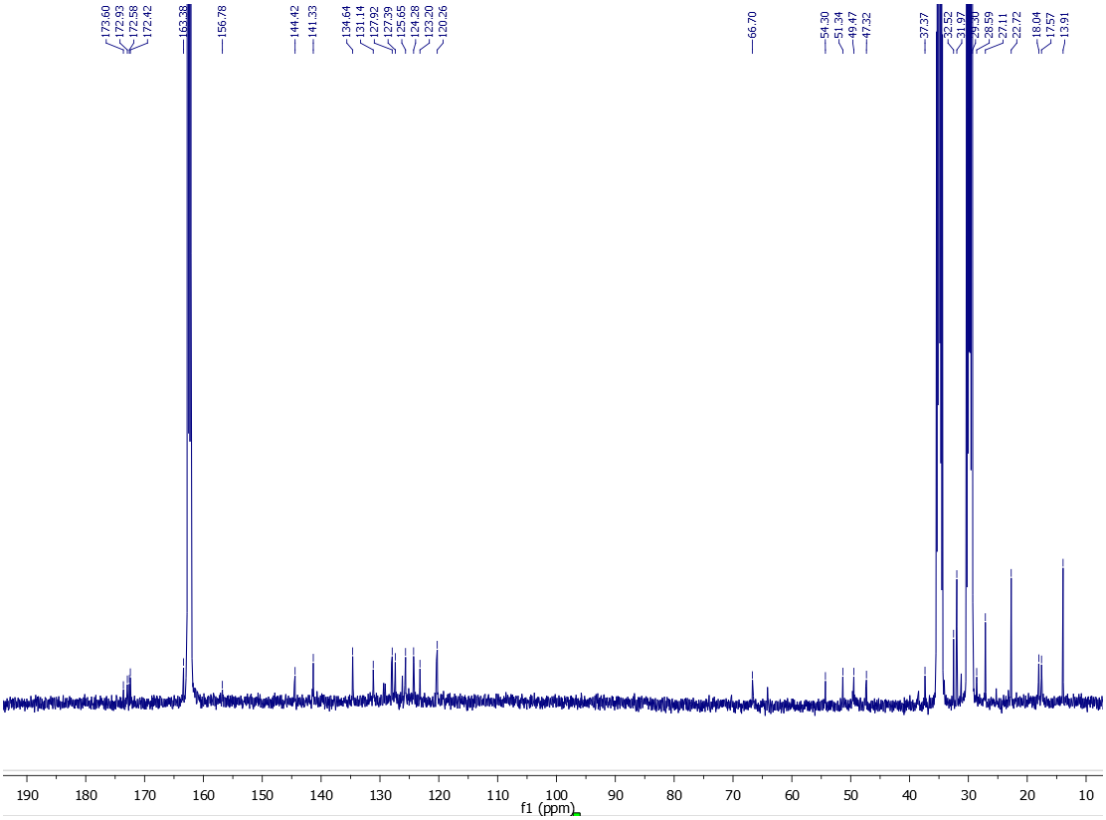
f1 (ppm)

Compound **6**





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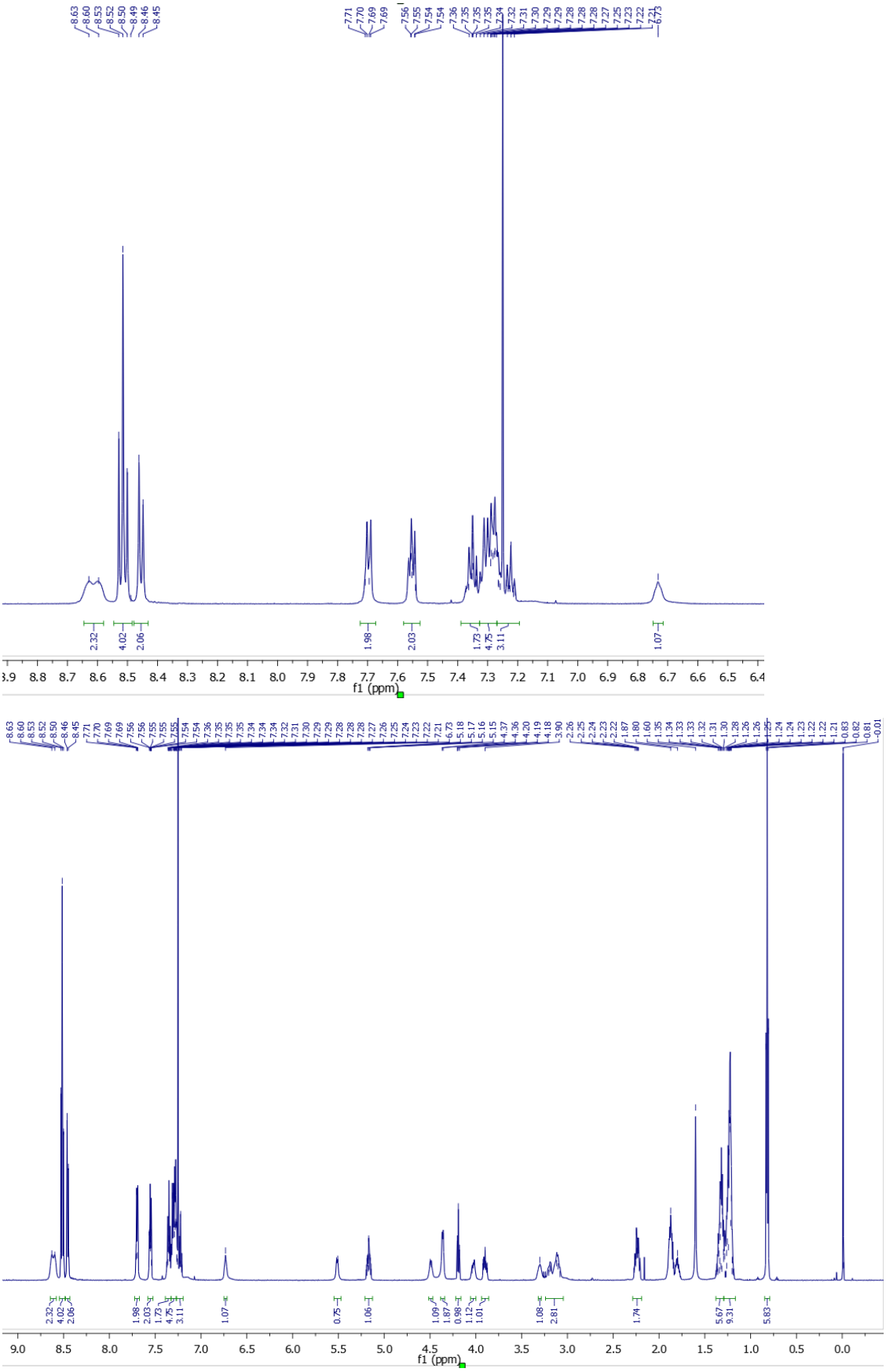

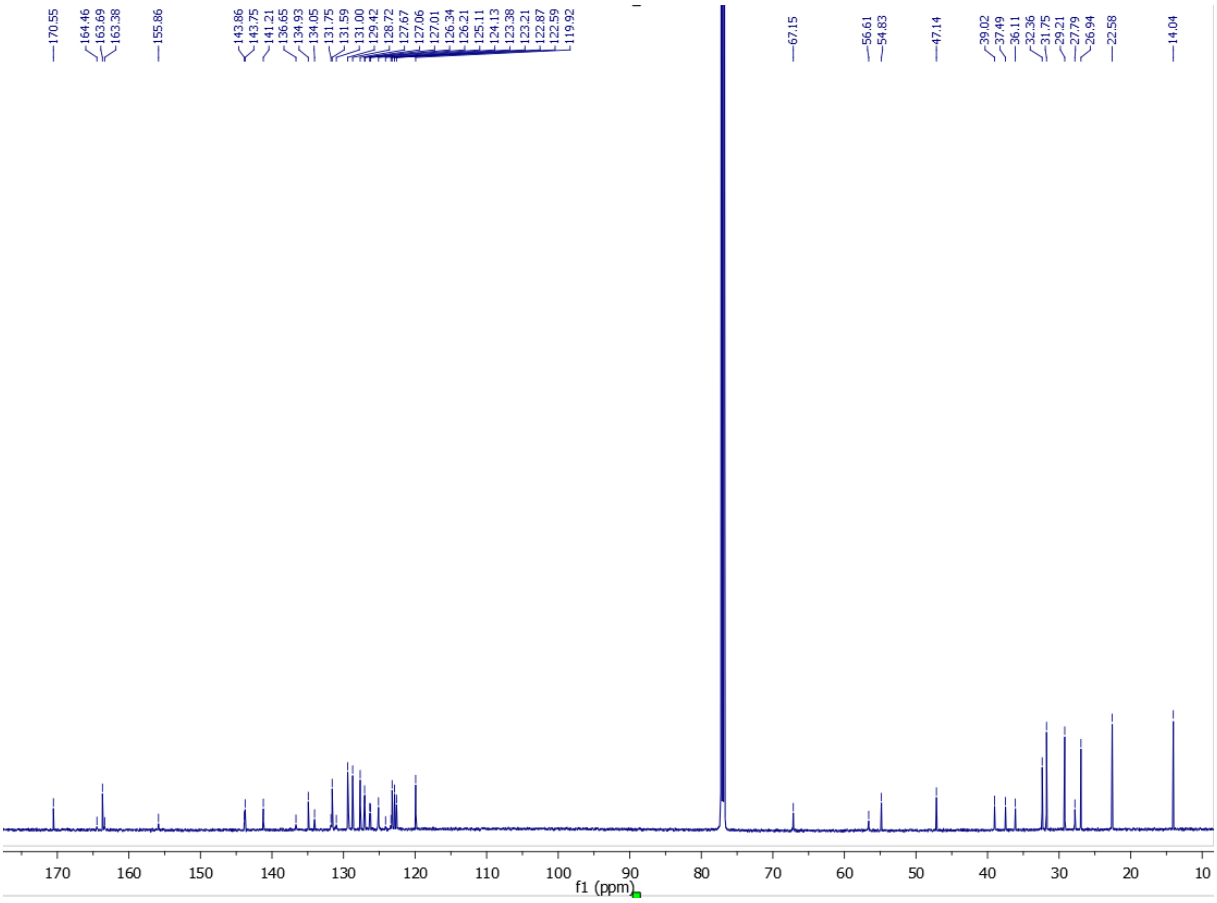
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26.94
22.58
14.04
170
160
150
140
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100
90
80
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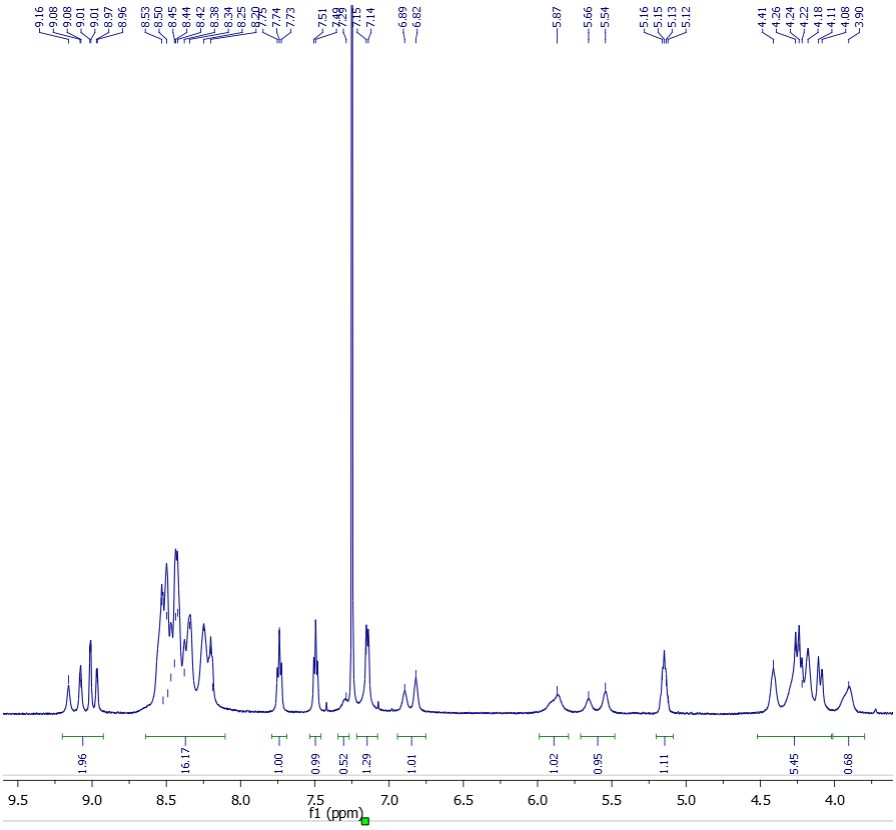
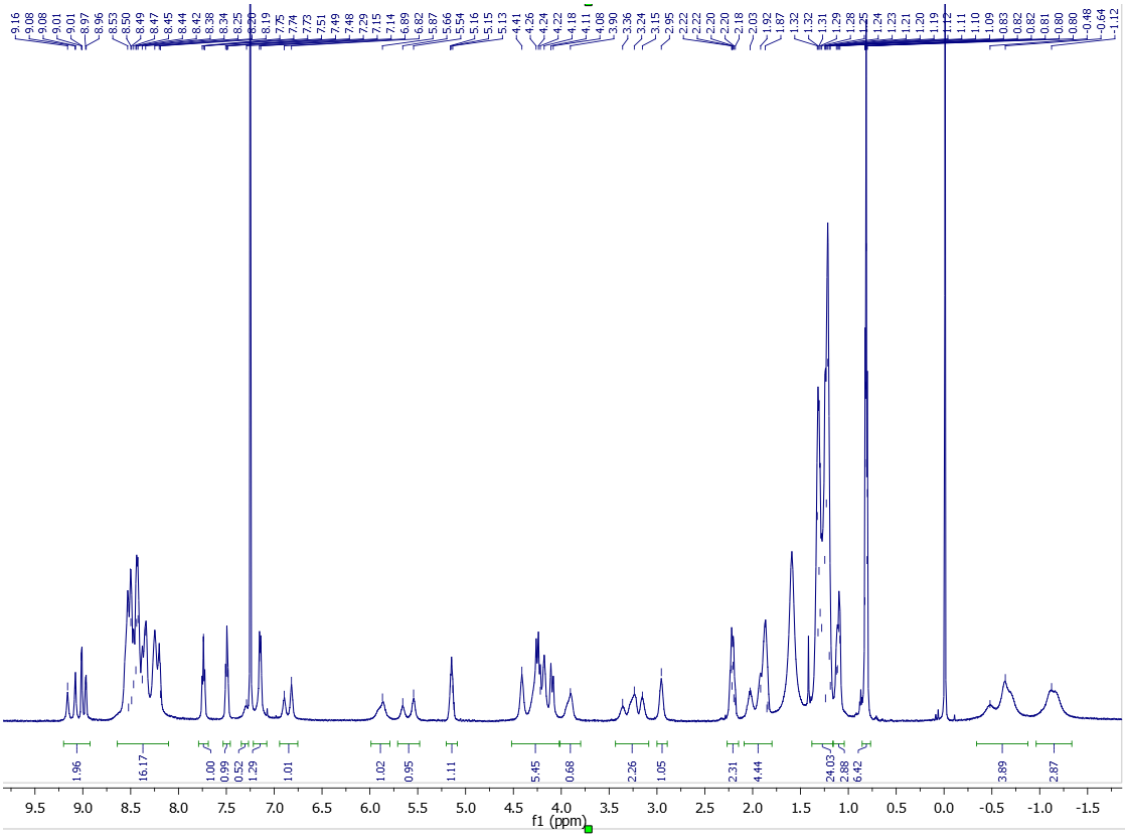
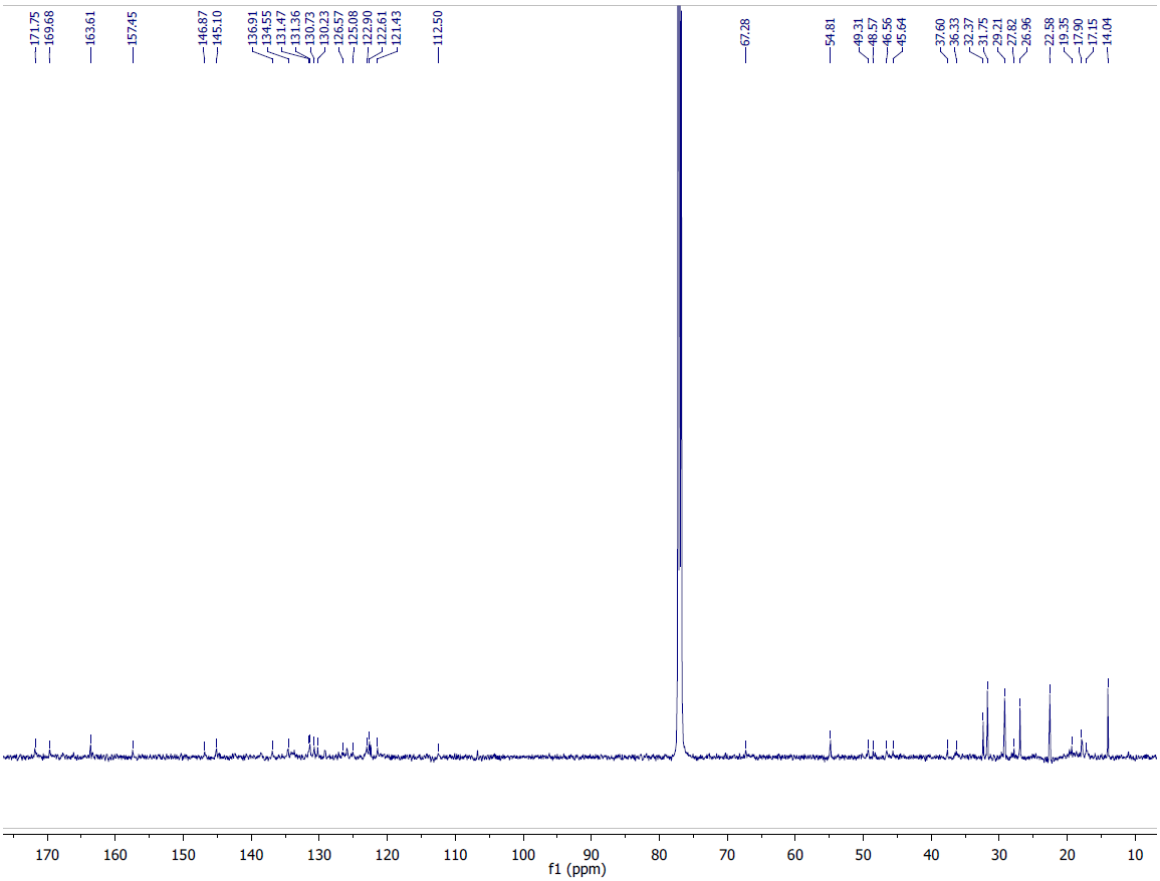
20
10
f1 (ppm)

Cor-(Ala)$_4$-PDI



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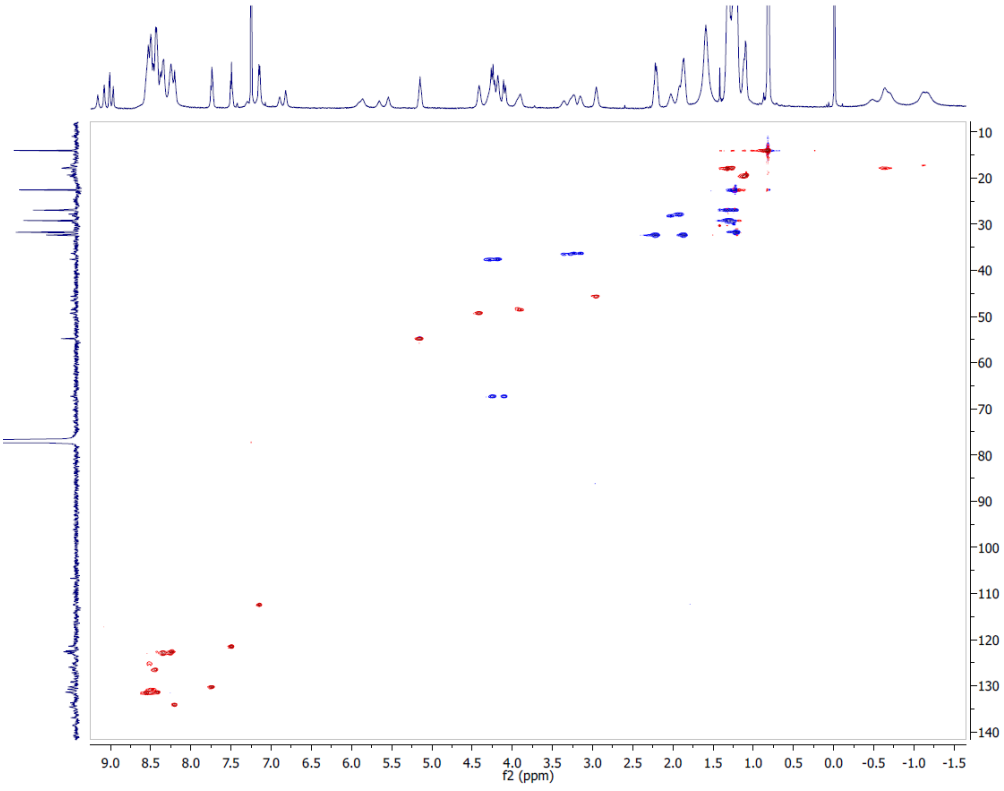
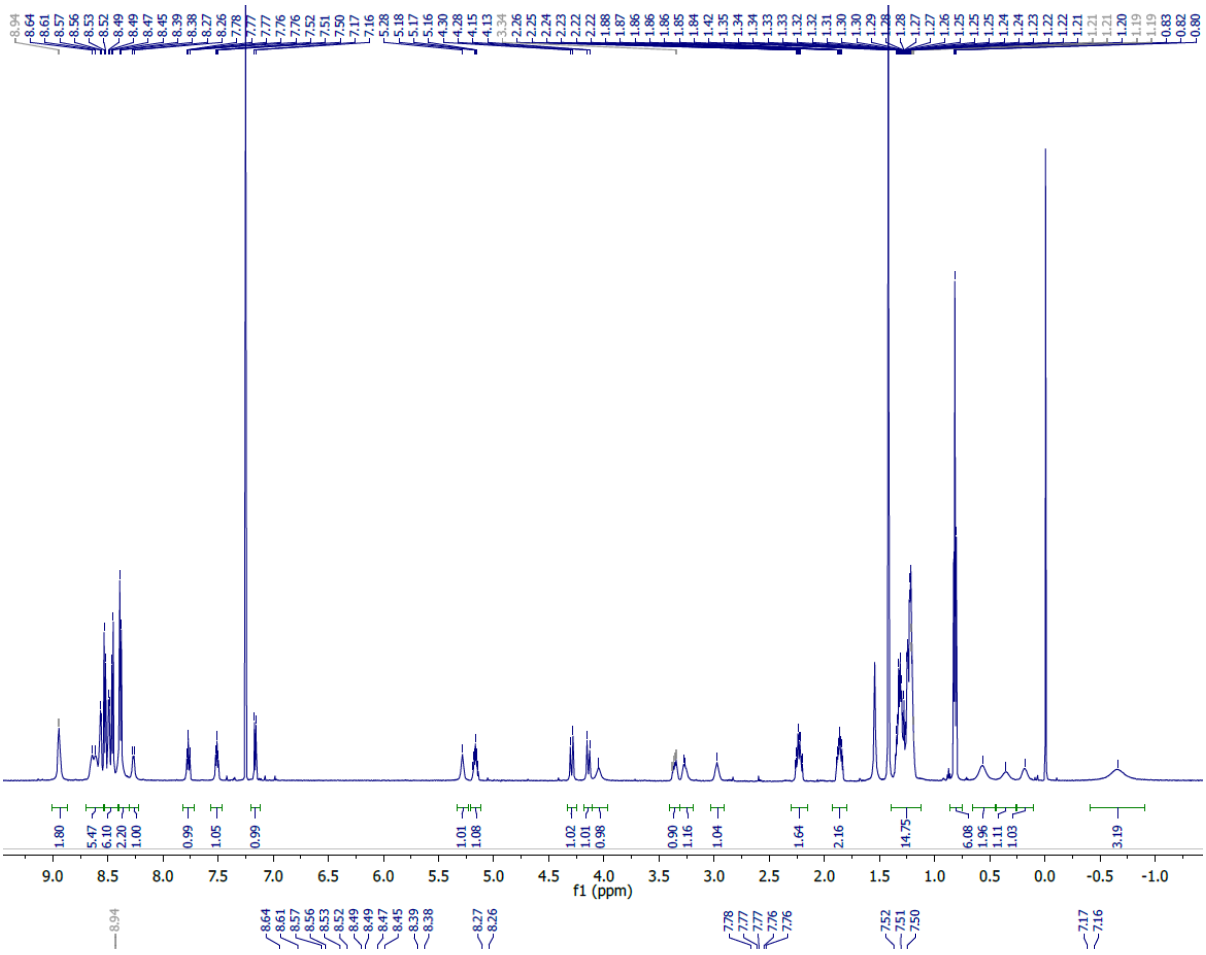
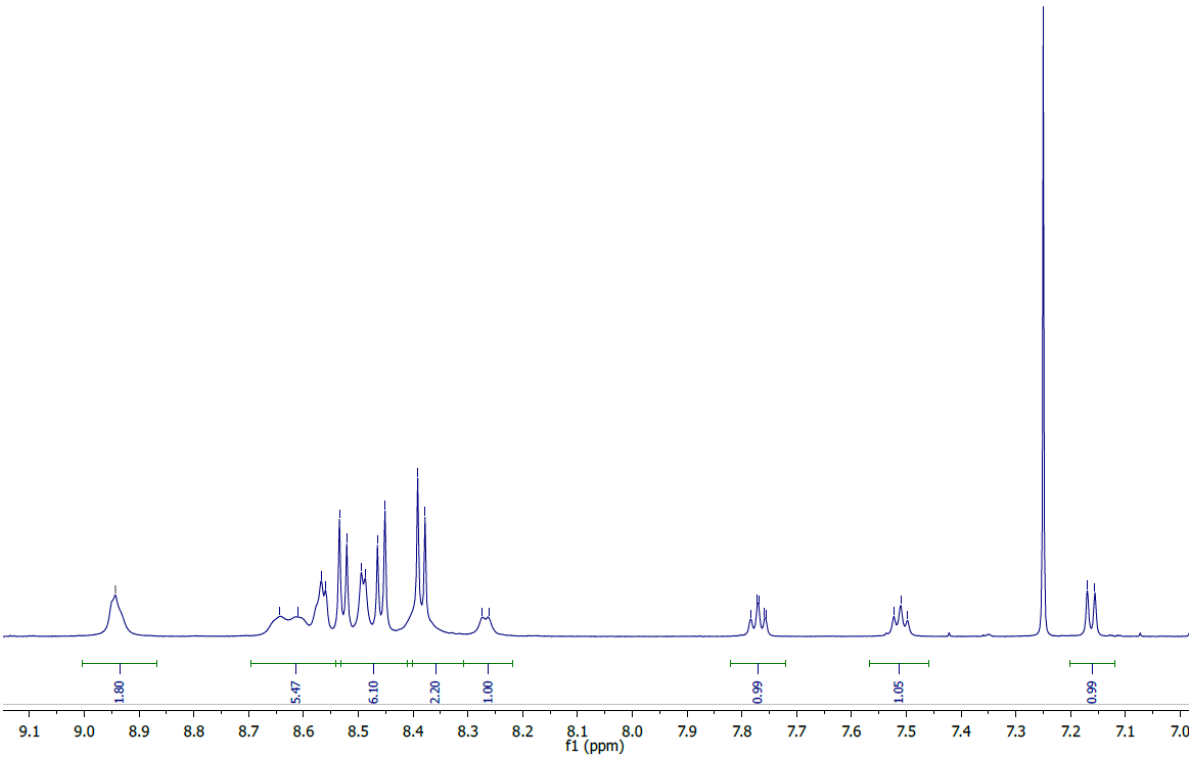
f1 (ppm)

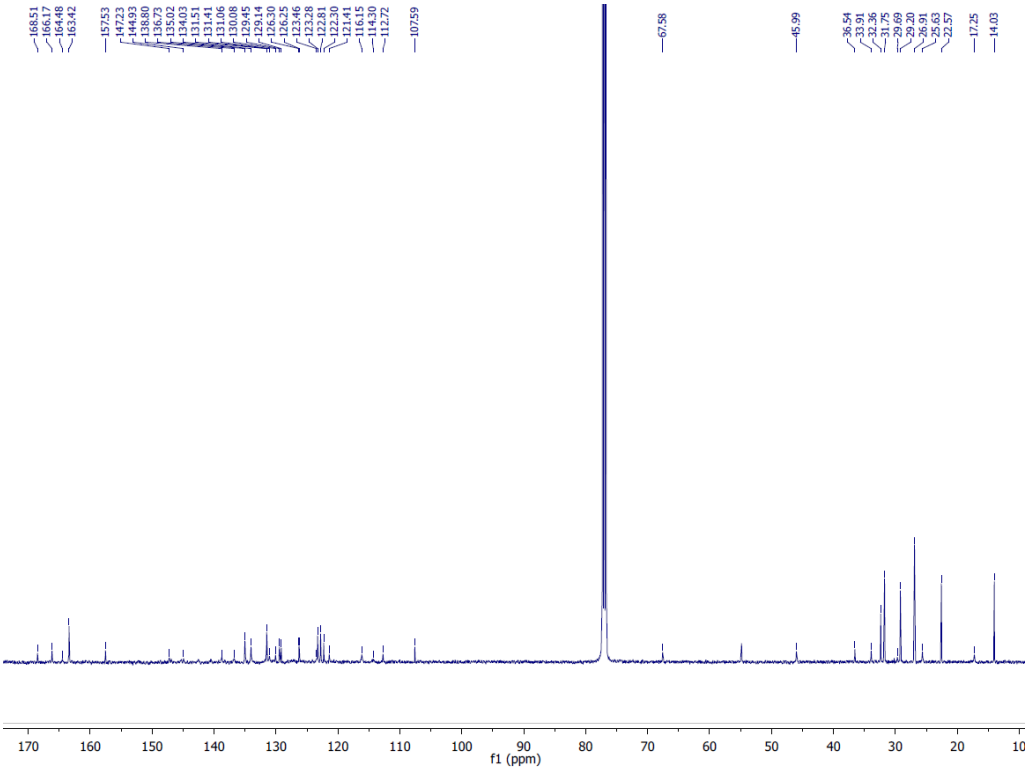
^{1}H-^{13}C HSQC


f2 (ppm)

Cor-Ala-PDI



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121.41
116.15
114.30
112.72
107.59
67.58
45.99
36.54
33.91
32.36
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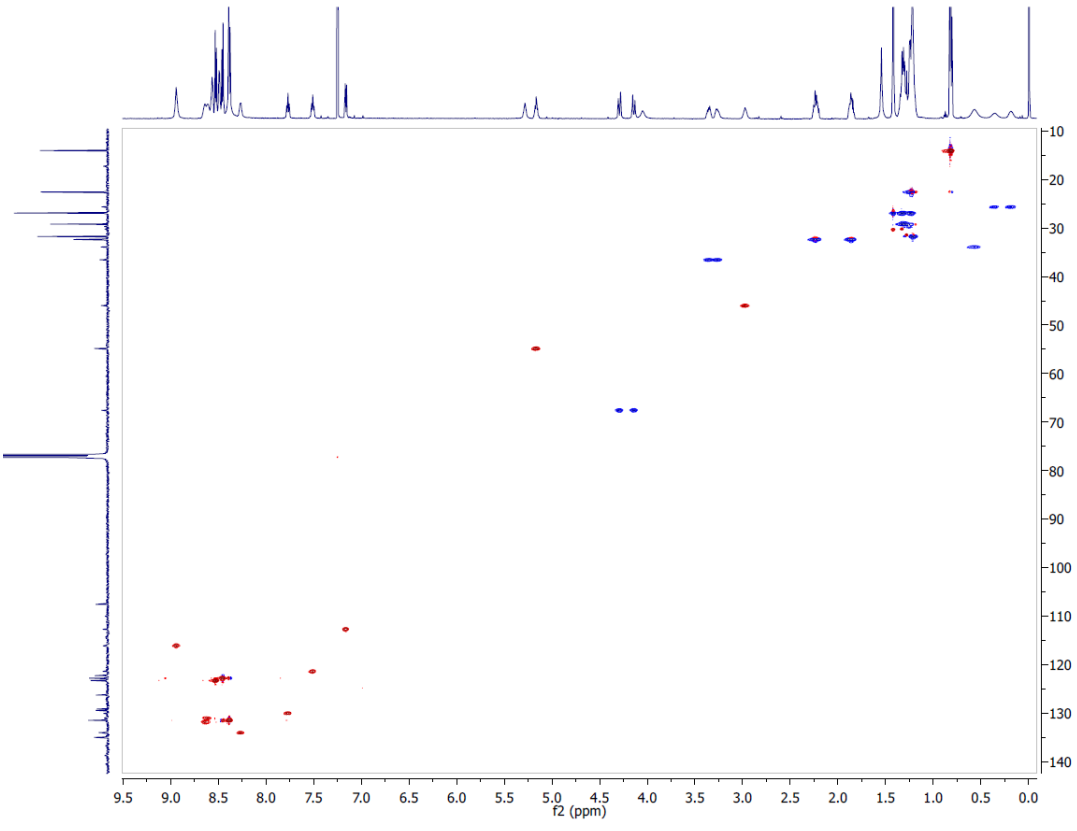
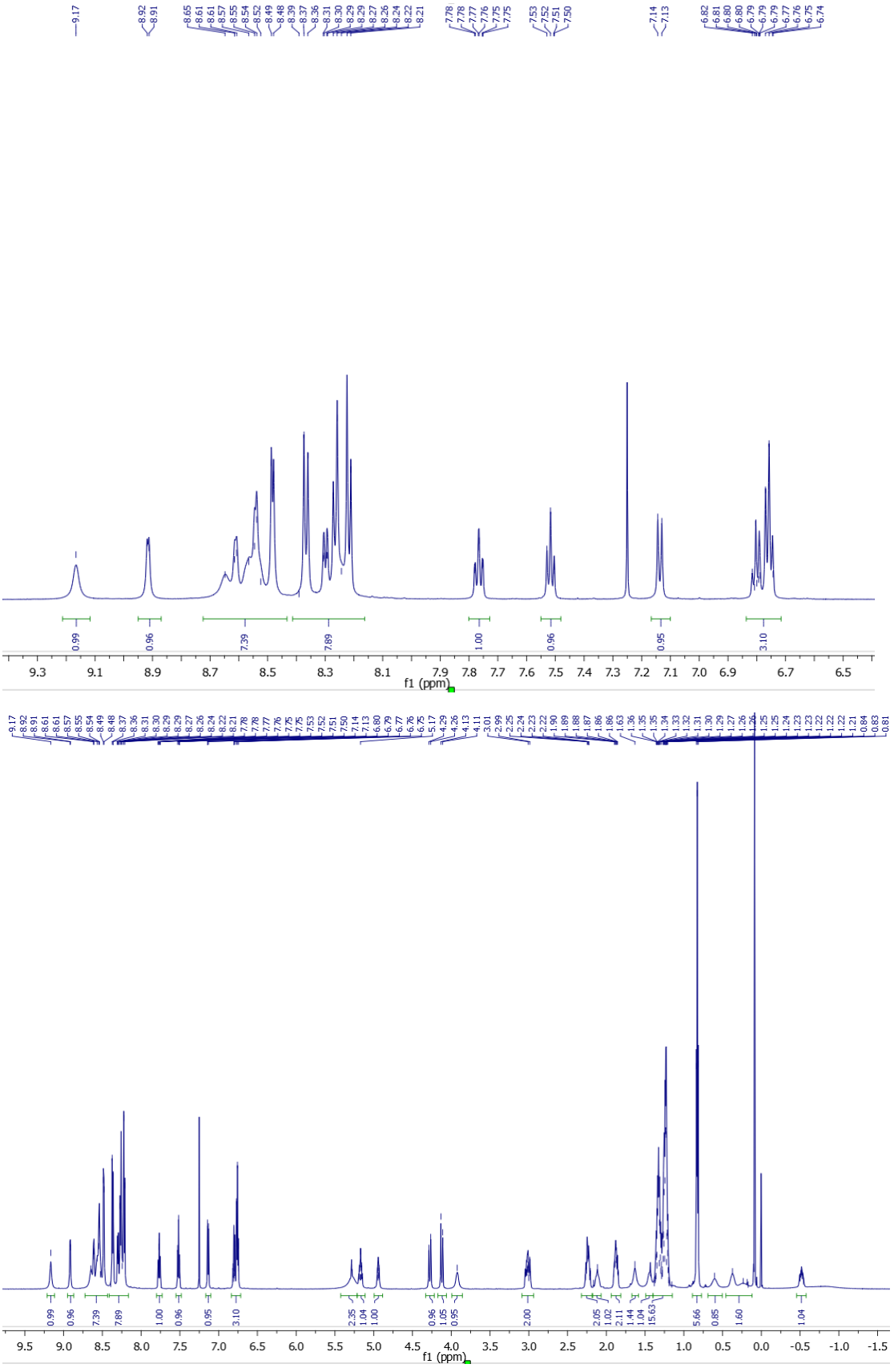
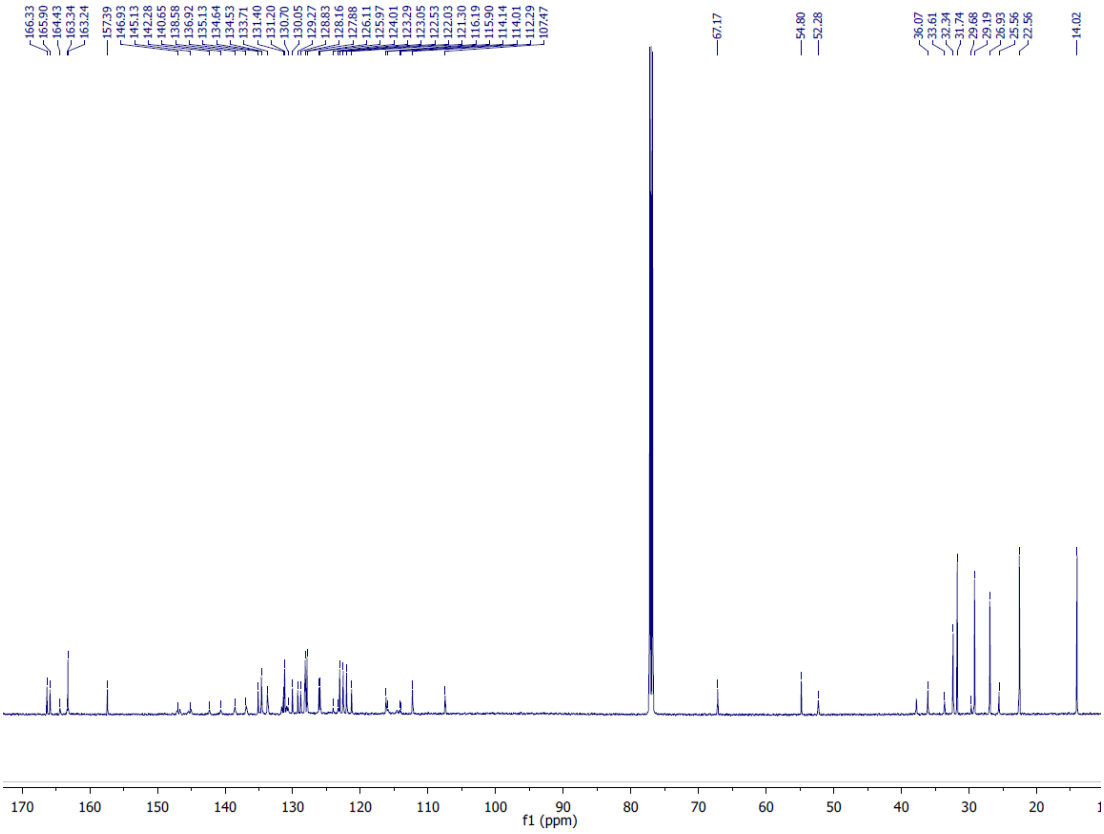
29.20
26.91
25.63
22.57
17.25
14.03
f1 (ppm)

^{1}H-^{13}C HSQC


f2 (ppm)

Cor-Phe-PDI

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116.19
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107.47
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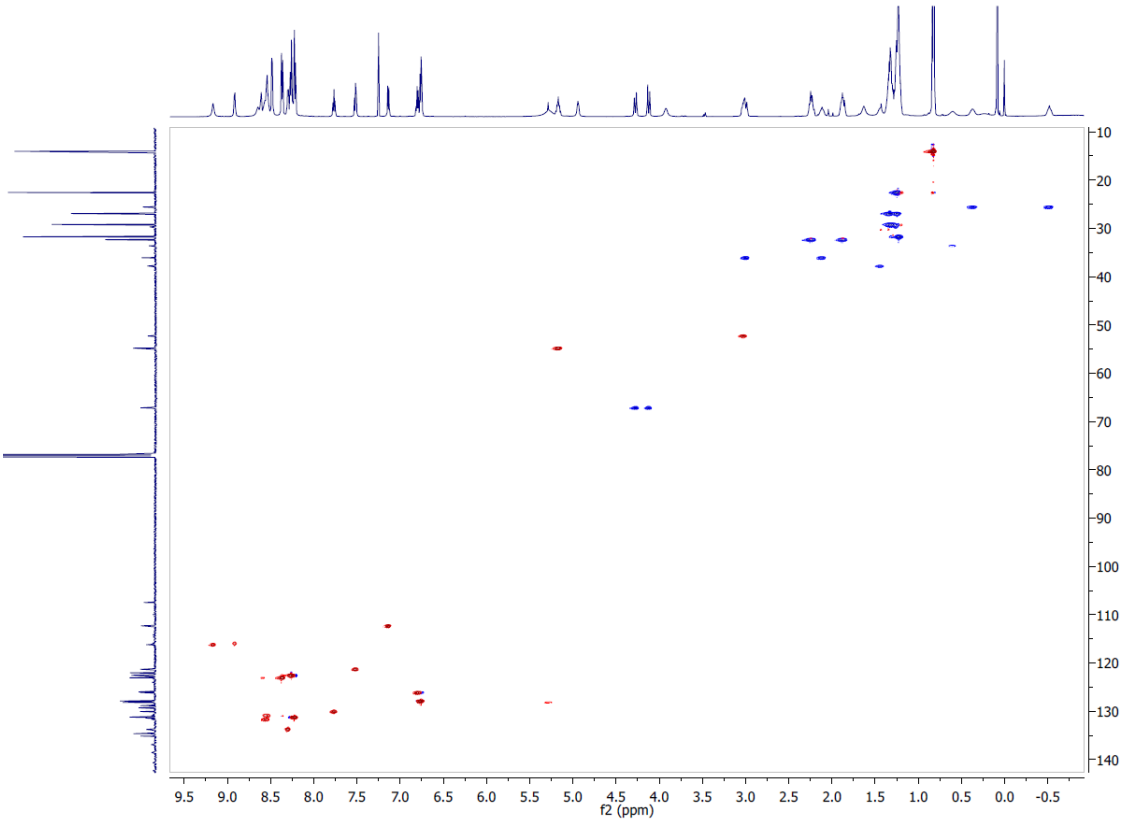
f1 (ppm)

^{1}H-^{13}C HSQC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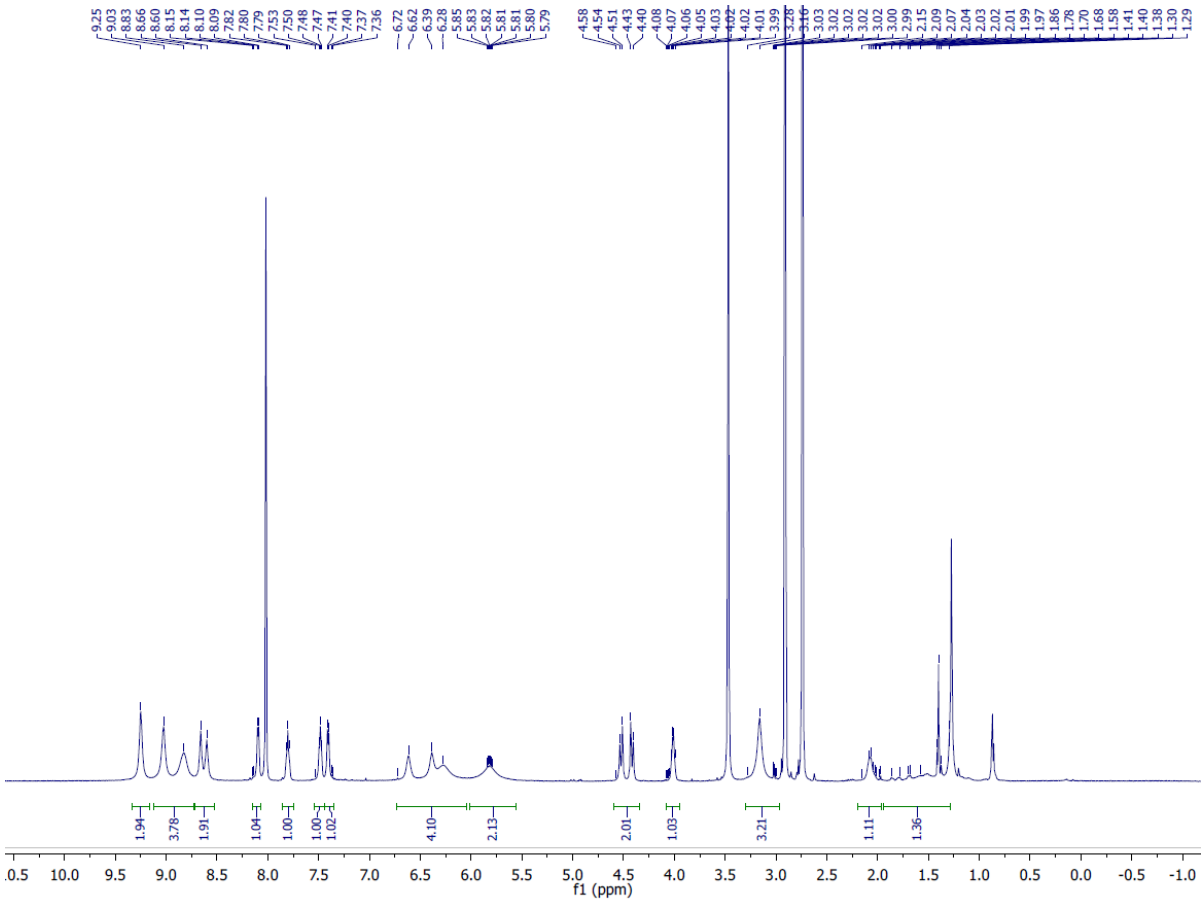
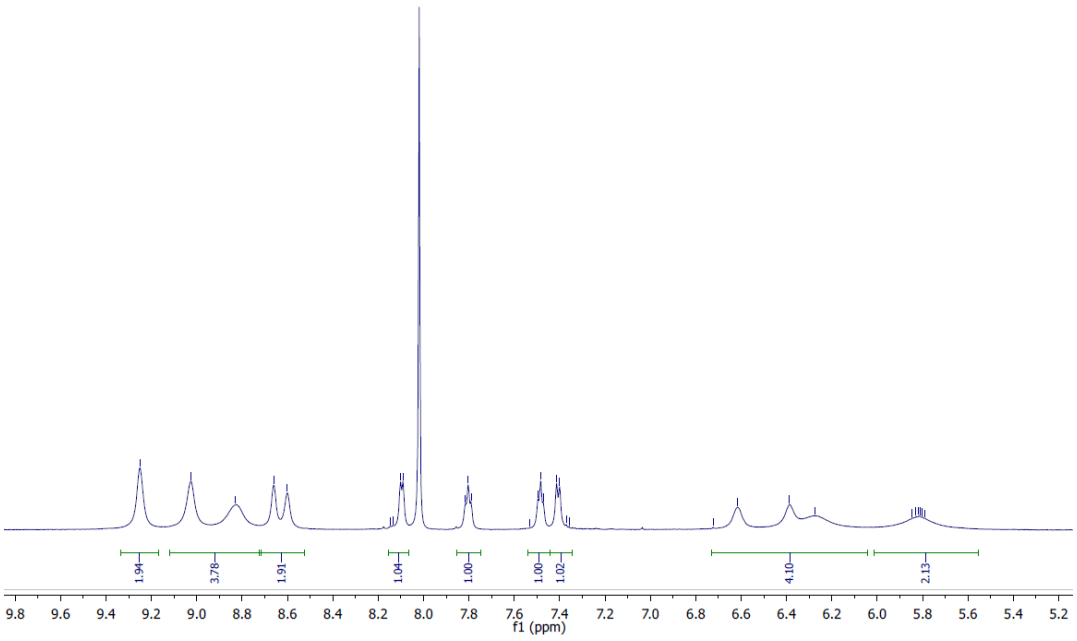
f2 (ppm)

Cor-Phe





3. Electrochemical analysis

3.1. Cyclic voltammetry (CV). CV measurements were performed using three-electrode cells powered by: (1) Bio-Logic SP-50 potentiostat (Lambda System, Warsaw, Poland); and (2) Reference 600 potentiostat-galvanostat (Gamry Instruments, Warminster, PA, USA). We utilized a glassy carbon working electrode for Cor oxidation and a platinum working electrode for PDI reduction, along with platinum counter electrodes. A high-impedance Ag/AgCl (3.0 M NaCl) electrode and an SCE electrode, connected to the cell via an electrolyte bridge containing 100 mM (n-$C_4H_9)_4NPF_6$ in acetonitrile (MeCN), served as references. Anhydrous MeCN, benzonitrile and dichloromethane were employed with different concentrations, C_{el}, of a supporting electrolyte ($N(C_4H_9)_4PF_6$), ranging from 25 mM to 200 mM with 25-mM increments. Immediately before and immediately after each set of measurements for a solvent with different C_{el}, we record the CVs of ferrocene in acetonitrile in the presence of 100 mM $N(C_4H_9)_4PF_6$ in order to correct should potential drifts of the reference electrodes occur.[3, 4] Prior to each measurement, the sample was purged with argon. These experiments were carried out at room temperature at a scan rate of 100 $mV \cdot s^{-1}$. For each sample, we recorded a triplicate of measurements.

3.2. Voltammogram analysis. The mean of the cathodic and anodic peak potentials provides estimates for the half-wave potentials, $E^{(1/2)}$, from voltammograms that show chemical reversibility and even partial reversibility.[4] The zero values of the first derivatives of the voltammograms provide estimates for the peak potentials, i.e., the potentials where $\partial I/\partial E = 0$, while $\partial E/\partial t$ = constant [5]. For irreversible oxidation and reduction, the potentials at the inflection points of the anodic and cathodic waves, respectively, extracted from the zero values of the second derivatives of the voltammograms, provide estimates for $E^{(1/2)}$, i.e., the potentials where $\partial^2 I/\partial E^2 = 0$, while $\partial E/\partial t$ = constant [4, 5]. The dependence of $E^{(1/2)}$ on the electrolyte concertation, C_{el}, allows extrapolating to $C_{el} = 0$ and estimating the values of the reduction potentials for neat solvent, $E_0^{(1/2)}$ (Figure 5b).([3,4]) For each solvent, we estimate $\Delta E_0^{(1/2)} = E_0^{(1/2)}{}_{Cor^{+\bullet}|Cor} - E_0^{(1/2)}{}_{PDI|PDI^{-\bullet}}$. The linear dependence of $\Delta E_0^{(1/2)}$ on the inverse of the relative dielectric constants, ε^{-1} (eq. 3b), yields $\Delta E_0^{(1/2)}$ for toluene ($\varepsilon^{-1} = 0.42$) and $S_{1/r}$, which we use for estimating the CT driving forces (eq. 3a) and the medium reorganization energy (Figure 5d).

4. Steady-state optical spectroscopy

4.1. Absorption and emission. The optical absorption spectra were recorded using a Varian Cary 50 UV-vis and Jasco V-660 UV-vis-NIR spectrophotometer. Fluorescence measurements were conducted with a Horiba Jobin Yvon Fluorolog-3-22 spectrofluorometer. All samples were purged with argon prior to measurement. The absorbance at the excitation wavelengths was kept within the range between 0.1 and 0.2 for measurements of the emission quantum yields. 10-[2-(N-butylcarbamoylmethoxy)phenyl]-5,15-bis(pentafluorophenyl)corrol (ϕ_{fl} = 0.134, for MeOH) was used as a standard. [5]

4.2. Estimating the inner reorganization energy (λ_v). The fluorescence spectra of **PDI** and **Cor** in toluene (T = 295 K) were modeled using a semiclassical Franck-Condon expression with one classical distortion and one quantum mechanical distorting mode.[6, 7] The vibrational frequencies of the distorting mode were assumed to be identical in the ground and excited electronic states. The classical-mode distortion was represented by a Gaussian function with FWHM (cm^{-1}) $\approx [2274 \times \lambda_{classical}\ (cm^{-1})]^{1/2}$. The energy maximum of the Gaussian for the transition from the quantum mechanical vibrationally unexcited ground electronic state to the quantum mechanical vibrationally unexcited luminescent electronic state is defined as the parameter E_{00}. Distortions in the quantum mechanical vibrational mode of frequency ν are described by the Haung-Rhys parameter, S. The model parameters derived for **PDI** are: E_{00} = 18475 cm^{-1}; $h\nu$ = 1270 cm^{-1}; S = 0.82; $\lambda_{classical}$ = 300 cm^{-1} (**Figure S1**). The model parameters derived for **Cor** are: E_{00} = 15250 cm^{-1}; $h\nu$ = 1250 cm^{-1}; S = 0.32; $\lambda_{classical}$ = 350 cm^{-1} (**Figure S1**). The estimated upper limit to the inner-sphere reorganization is $\lambda_{inner} \leq (S \times h\nu) + \lambda_{classical}$: λ_{inner}(**PDI**) ≤ 0.17 eV; λ_{inner}(**Cor**) ≤ 0.09 eV.

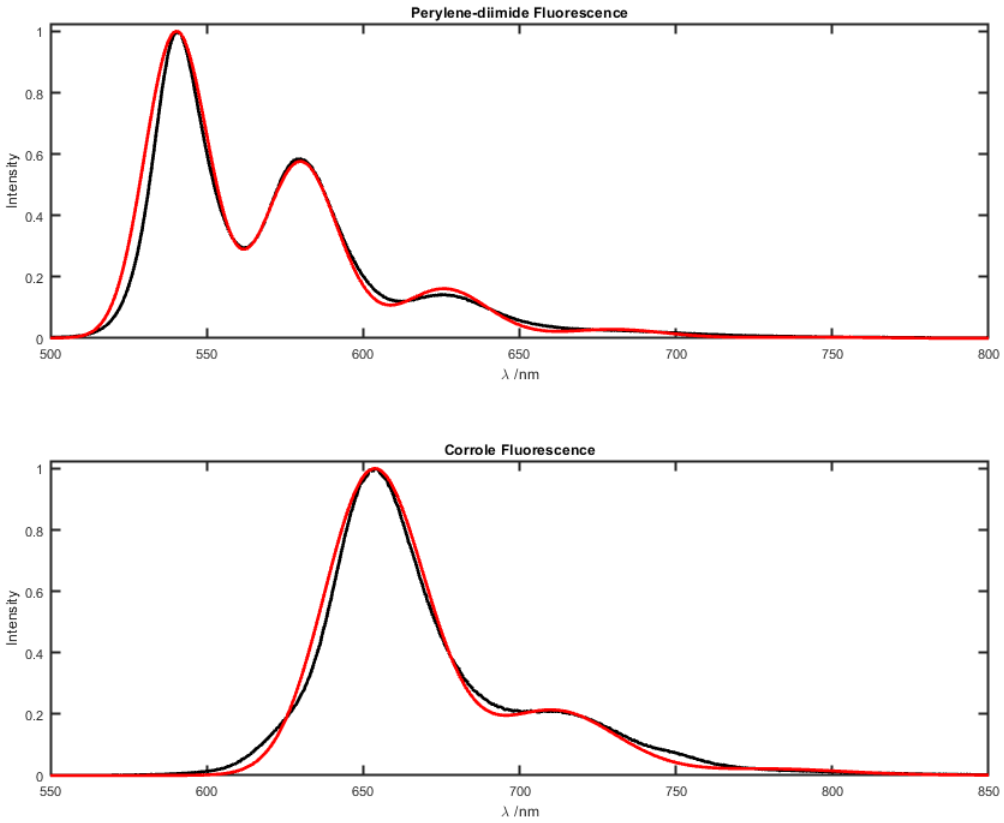


Figure S1. Measured (black) and modeled (red) fluorescence spectra of **PDI** and **Cor**. See text for model parameters.

4.3. Circular dichroism. The ECD spectra of for **Cor-(Ala)$_4$-PDI**, **Cor-Ala-PDI**, and **Cor-Phe-PDI** were recorded between 700 and 280 nm at room temperature in spectroscopic grade toluene with concentrations in the range from 5.94×10^{-5} to 6.83×10^{-5} M in a 0.1-cm quartz cell.

5. Time-resolved optical spectroscopy

5.1. Time-resolved fluorescence spectroscopy. The 1064-nm output of a passively mode-locked Nd:YAG laser (Spectra Physics Vanguard) was regeneratively amplified (Continuum) and frequency tripled using KDP crystals to produce 355-nm excitation pulses (~10 ps, 10 Hz). Luminescence was collected 90° from the excitation, passed through a polarizer oriented at the magic angle, then directed onto the entrance slit of a monochromator for wavelength selection. Fluorescence decays were measured using a streak camera (Hamamatsu C5680) in photon-counting mode, and data were collected with 1-, 10-, or 20-ns time windows. Instrument response time is ~1-2% of the time window. Samples were prepared in sealed 1 cm quartz cuvettes under Ar and were stirred during data acquisition.

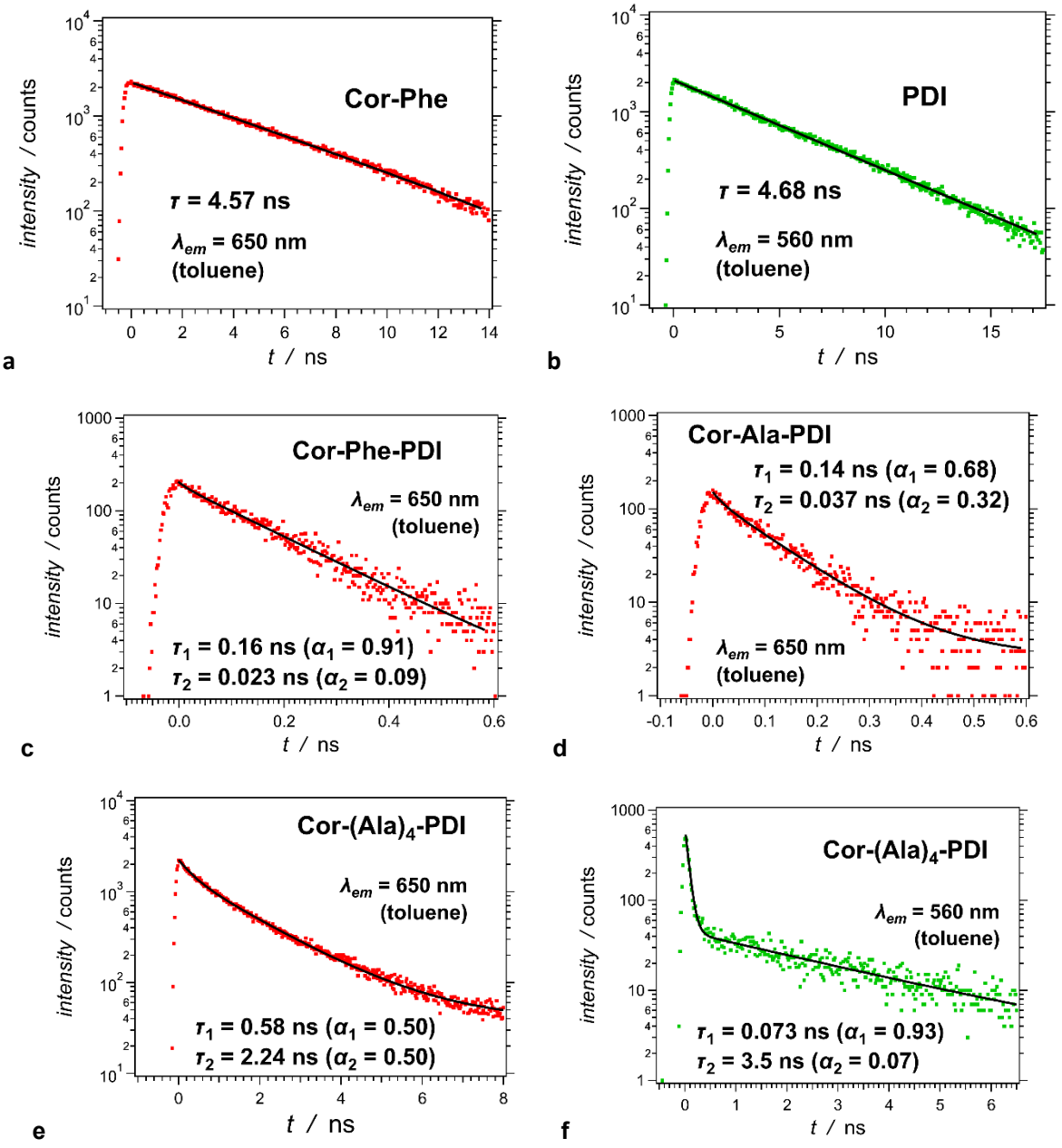


Figure S2. Emission decays with the corresponding exponential data fits (solid lines). Cor-Phe and PDI decays were adequately described by single-exponential functions. Biexponential functions were necessary to describe the decays of the Cor-PDI DBA conjugates. Time constants (τ_i) and amplitudes (α_i) for each phase are indicated pm the plots.

5.2. Transient-absorption (TA) spectroscopy. A Helios pump-probe spectrometer (Ultrafast Systems, LLC, Florida, USA) was used to carry out TA measurements recorded in a transmission mode. 800-nm pulses (≥35 fs, 4.0 mJ per pulse, at 1 kHz) were generated by a SpitFire Pro 35F regenerative amplifier (Spectra Physics, Newport, CA, USA). The amplifier was pumped with an Empower 30 Q-switched laser ran at 20 W. A MaiTai SP oscillator provided the seed beam (55 nm bandwidth). The wavelength of the pump was tuned using an optical parametric amplifier, OPA-800CU (Newport Corporation, Newport, CA, USA), equipped with harmonic generators. Responses from pure solvents were used for the chirp correction of the TA data. The data analysis was carried out using Surface Xplorer (Ultrafast Systems, LLC, Florida, USA) and IgorPro v. 8 (WaveMetrics, Inc., Lake Oswego, OR, USA).[8-10]

Steady-state optical absorption spectra reveal that when exciting the DBA conjugates at 400 to 430 nm, the electron donor, Cor, absorbs more than 95% of the light. When exciting the DBA conjugates at 460 to 470 nm, the electron acceptor, PDI, absorbs about 90% of the light. These results justify the use of 400 nm pump for selective excitation of the electron donor, and 465 nm pump for selective excitation of the electron acceptor.

5.3. Kinetic analysis. To analyze the TA dynamics, we use global fits employing sums of exponential functions:

$$\Delta A(\lambda, t) = Б_{\mathrm{CT}}(\lambda)\, \Delta A_{\mathrm{CT}}(\lambda, t) + Б_{\mathrm{LEC}}(\lambda)\, \Delta A_{\mathrm{LEC}}(\lambda, t) + Б_{\mathrm{BC}}(\lambda)\, \Delta A_{\mathrm{BC}}(\lambda, t) + Б_{\mathrm{LEP}}(\lambda)\, \Delta A_{\mathrm{LEP}}(\lambda, t) + Б_{\mathrm{BP}}(\lambda)\, \Delta A_{\mathrm{BP}}(\lambda, t) \tag{S1}$$

Where each term, $Б_i(\lambda)\, \Delta A_i(\lambda, t)$, represents species that have the same TA dynamics, with amplitudes from the signals scaled by $Б_i(\lambda)$.

The charge-transfer (CT) term depicts the rise (via ET and HT) and the decay (via CR) of the TA of the radical ions:

$$\Delta A_{\mathrm{CT}}(\lambda, t) = -\sum_{i=1}^{p} \alpha_i^{(\mathrm{HT})}(\lambda)\, e^{-k_i^{(\mathrm{HT})} t} - \sum_{i=1}^{n} \alpha_i^{(\mathrm{ET})}(\lambda)\, e^{-k_i^{(\mathrm{ET})} t} + \sum_{i=1}^{w} \alpha_i^{(\mathrm{CR})}(\lambda)\, e^{-k_i^{(\mathrm{CR})} t} \tag{S2a}$$

where $\Sigma_i\, \alpha_i^{(\mathrm{HT})} + \Sigma_i\, \alpha_i^{(\mathrm{ET})} = \Sigma_i\, \alpha_i^{(\mathrm{CR})}$. The terms in the first sum depict HT, Cor···^{1}PDI* → Cor$^{\bullet+}$···PDI$^{\bullet-}$, in the second sum – ET, ^{1}Cor*···PDI → Cor$^{\bullet+}$···PDI$^{\bullet-}$, and in the third sum – CR, Cor$^{\bullet+}$···PDI$^{\bullet-}$ → Cor···PDI.

The term for the Cor locally excited state (LEC) describes the dynamics of ^{1}Cor*, that, in addition to the initial amplitude, $\Delta A_{\mathrm{LEC}}(\lambda, 0) = \alpha_0^{(\mathrm{Cor})}$, due to direct excitation of Cor, gets populated by EnT from ^{1}PDI*, Cor···^{1}PDI* → ^{1}Cor*···PDI, and decays either directly to the ground state, ^{1}Cor* → Cor, or via ET, ^{1}Cor*···PDI → Cor$^{\bullet+}$···PDI$^{\bullet-}$ → Cor···PDI:

$$\Delta A_{\mathrm{LEC}}(\lambda, t) = -\sum_{i=1}^{m} \alpha_i^{(\mathrm{EnT})}(\lambda)\, e^{-k_i^{(\mathrm{EnT})} t} + \sum_{i=1}^{h} \alpha_i^{(\mathrm{Cor})}(\lambda)\, e^{-k_i^{(\mathrm{Cor})} t} \tag{S2b}$$

The first sum represents the EnT from ^{1}PDI*, and the second sum – the decay of ^{1}Cor*; also, $\Sigma_i\, \alpha_i^{(\mathrm{EnT})} + \alpha_0^{(\mathrm{Cor})} = \Sigma_i\, \alpha_i^{(\mathrm{Cor})}$; and $\alpha_i^{(\mathrm{EnT})} \propto \alpha_i^{(\mathrm{PDI})}\, k_i^{(\mathrm{EnT})} / (k_i^{(\mathrm{EnT})} + k_i^{(\mathrm{HT})} + k_0^{(\mathrm{PDI})})$

The rate constants, $k_i^{(\mathrm{Cor})}$, encompass all modes of deactivation of ^{1}Cor*, i.e., $k_i^{(\mathrm{Cor})} = k_i^{(\mathrm{ET})} + k_0^{(\mathrm{Cor})}$, where $k_0^{(\mathrm{Cor})}$ is cumulative for the pathways of ^{1}Cor* deactivation that do not involve the PDI moiety, as obtained from the time-resolved fluorescence analysis of **Cor-Phe**, $k_0^{(\mathrm{Cor})} = 2.2\times10^8$ s^{-1} (Figure S2a). The $\alpha_i^{(\mathrm{ET})}$ preexponential amplitudes of eq. S2b relate to $\alpha_i^{(\mathrm{Cor})}$ of eq. S2a, i.e., $\alpha_i^{(\mathrm{ET})} \propto (k_i^{(\mathrm{ET})} / k_i^{(\mathrm{Cor})})\, \alpha_i^{(\mathrm{Cor})}$.

$\Delta A_{\mathrm{LEC}}(\lambda, t)$ depicts the dynamics of the ^{1}Cor* TA between about 450 and 545 nm, and also in the red and NIR spectral region. This function, eq. S2b, with negative amplitudes, $-\Delta A_{\mathrm{LEC}}(\lambda, t)$, describes the stimulated emission (SE) of Cor in the TA spectra. In addition, for this analysis we multiply the fluorescence decay curves, recorded at 650 nm (Figure S2), by a negative constant for direct visual comparison with the SE TA traces.

The Cor bleach (BC) term describes the bleach enhancement (ΔA becoming more negative) and recovery (ΔA becoming more positive) originating, respectively, from the decrease and the increase in the ground-state absorption of Cor, which spreads throughout the visible region of the spectrum:

$$\Delta A_{\mathrm{BC}}(\lambda, t) = \sum_{i=1}^{m} \alpha'_i{}^{(\mathrm{PDI})}(\lambda)\, e^{-\left(k_i^{(\mathrm{EnT})} + k_i^{(\mathrm{HT})}\right) t} - \left(\sum_{i=1}^{w} \alpha_i^{(\mathrm{CR})}(\lambda)\, e^{-k_i^{(\mathrm{CR})} t} + \left(\sum_{i=1}^{n} \alpha'_i{}^{(\mathrm{Cor})}(\lambda) \right) e^{-k_0^{(\mathrm{Cor})} t} + \sum_{\substack{i=n+1 \\ [n>h-1] \Rightarrow \alpha_i^{(\mathrm{Cor})}=0}}^{h} \alpha_i^{(\mathrm{Cor})}(\lambda)\, e^{-k_i^{(\mathrm{Cor})} t} \right) \tag{S2c}$$

The first sum represents the EnT and HT from ^{1}PDI* that lead to removal of the S_0 state of Cor, where $\alpha'_i{}^{(PDI)} \propto \alpha_i^{(PDI)} (k_i^{(EnT)} + k_i^{(HT)}) / (k_i^{(EnT)} + k_i^{(HT)} + k_0^{(PDI)})$ (eq. S2d). The terms in the parentheses depict the deactivation of ^{1}Cor* and Cor$^{\bullet+}$ to ground state. The first sum in the parentheses shows the kinetics of the recovery of the Cor ground-state absorption from CR, as described in eq. S2a. The second sum encompasses the contributions from the inherent decay of ^{1}Cor* that is parallel with the ET steps, where $\alpha'_i{}^{(Cor)} \propto \alpha_i^{(Cor)} k_0^{(Cor)} / k_i$. The third term accounts for the deactivation of ^{1}Cor* to Cor that does not involve accumulation of the CT state. Indeed, when CR is faster than ET, ^{1}Cor*···PDI → Cor$^{\bullet+}$···PDI$^{\bullet-}$ → Cor···PDI becomes undiscernible from ^{1}Cor*···PDI → Cor···PDI, with ET the rate limiting step of this ET-CR deactivation.

The term for the PDI locally excited state (LEP) describes the dynamics of the locally excited state of the electron acceptor, ^{1}PDI*, that decays via EnT and HT, as well as via the inherent deactivation pathways, observed in the absence of Cor, characterized with $k_0^{(PDI)}$:

$$\Delta A_{LEP}(\lambda, t) = \sum_{i=1}^{m} \alpha_i^{(PDI)}(\lambda)\, e^{-\left(k_i^{(PDI)}\right) t} \qquad \text{(S2d)}$$

Where $k_i^{(PDI)} = k_i^{(EnT)} + k_i^{(HT)} + k_0^{(PDI)}$, and $k_0^{(PDI)} = 2.1\times10^8$ s^{-1} (Figure S2b).

$\Delta A_{LEP}(\lambda, t)$ depicts the decay of the ^{1}PDI* TA in the red and NIR spectral regions. The TA spectrum of ^{1}PDI* overlaps with the TA spectrum of PDI$^{\bullet-}$. The differences in the shapes TA bands and the extinction coefficients are relatively small, Nevertheless, they are sufficient to allow for discerning the dynamics of the CT species from that of the LE state of PDI. This function (eq. S2d) with negative amplitudes, $-F_{LEP}(\lambda, t)$, describes the stimulated emission, SE of PDI, appearing between about 500 nm to 650 nm. In addition, for the analysis of **Cor-(Ala)$_4$-PDI**, with λ_{ex} = 465 nm, we multiply the fluorescence decay curves, recorded at 560 nm (Figure S2f), by a negative constant for direct visual comparison with the SE TA traces.

The PDI bleach (BP) term describes the bleach recovery of the ground-state absorption of PDI, which extends to about 550 nm into the visible spectral region:

$$\Delta A_{BP}(\lambda, t) = -\sum_{i=1}^{m} \alpha''_i{}^{(PDI)}(\lambda)\, e^{-\left(k_i^{(EnT)} + k_0^{(PDI)}\right) t} + \left(\sum_{i=1}^{n} \alpha_i^{(ET)}(\lambda)\, e^{-k_i^{(ET)} t} - \sum_{i=1}^{w} \alpha_i^{(CR)}(\lambda)\, e^{-k_i^{(CR)} t}\right) \qquad \text{(S2e)}$$

The first sum represents the bleach recovery from the deactivation of ^{1}PDI* via EnT, and via the radiative and non-radiative decays that do not involve the Cor moiety; $\alpha''_i{}^{(PDI)} \propto \alpha_i^{(PDI)} (k_i^{(EnT)} + k_0^{(PDI)}) / (k_i^{(EnT)} + k_i^{(HT)} + k_0^{(PDI)})$. The terms in the parentheses account for the CT processes, i.e., the PDI bleach enhancement resulting from ET, and the bleach recovery due to CR.

For excitation of the donor at 400 nm, we set $B_{LEP} = B_{BP} = 0$ (eq. S1), $\alpha_i^{(PDI)} = \alpha'_i{}^{(PDI)} = \alpha''_i{}^{(PDI)} = 0$, and $k_i^{(HT)} = k_i^{(EnT)} = k_0^{(PDI)} = 0$ (eq. S2). Global analysis employing this model (eq. S1 and S2) allows fitting the TA data and the fluorescence decays of **Cor-Ala-PDI** and **Cor-Phe-PDI** using five exponential components, i.e., $n = h = 3$ and $w = 2$, eq. S2 (Figure S3a,b, Table 1). Increasing the number of exponential terms yields rate constants, k_i, with closely similar values and no improvement of the fits. Still, the multiexponential outcomes from this analysis are consistent with the conformational heterogeneity of the conjugates that modulates not only the charge-separation (CS) but also the CR kinetics.

To attain good fits for **Cor-(Ala)$_4$-PDI**, the same global analysis, using eq. S1 and S2, resorts to five exponential components for the ^{1}Cor* deactivation, i.e., $h = 5$ (eq. S2b,c). Four of the five components describe the kinetics of the formation of the CT state, i.e., $n = 4$ (eq. S2a,c). The fifth component depicts a direct deactivation of ^{1}Cor* to ground state, corresponding to conformers that do not efficiently mediate ET, i.e., $k_5^{(ET)} << k_5^{(Cor)} \approx k_0^{(Cor)}$ (eq. S2, Figure S3c, Table 1). Biexponential decay of the CT state described well the CR dynamic, i.e., $w = 2$ (eq. S2) (Figure S3c, Table 1).

The three components describing the fastest ET, are similar for all three conjugates (Table 1). This feature suggests for close similarity between the donor-acceptor electronic-coupling pathways in the

three conjugates, regardless the length of the linker and the size of the side chains of the amino acids. The larger length of the flexible bridge in **Cor-(Ala)$_4$-PDI**, in comparison to that of the other two DBA conjugates, increases the degrees of freedom and leads to conformers that do not mediate ET as efficiently.

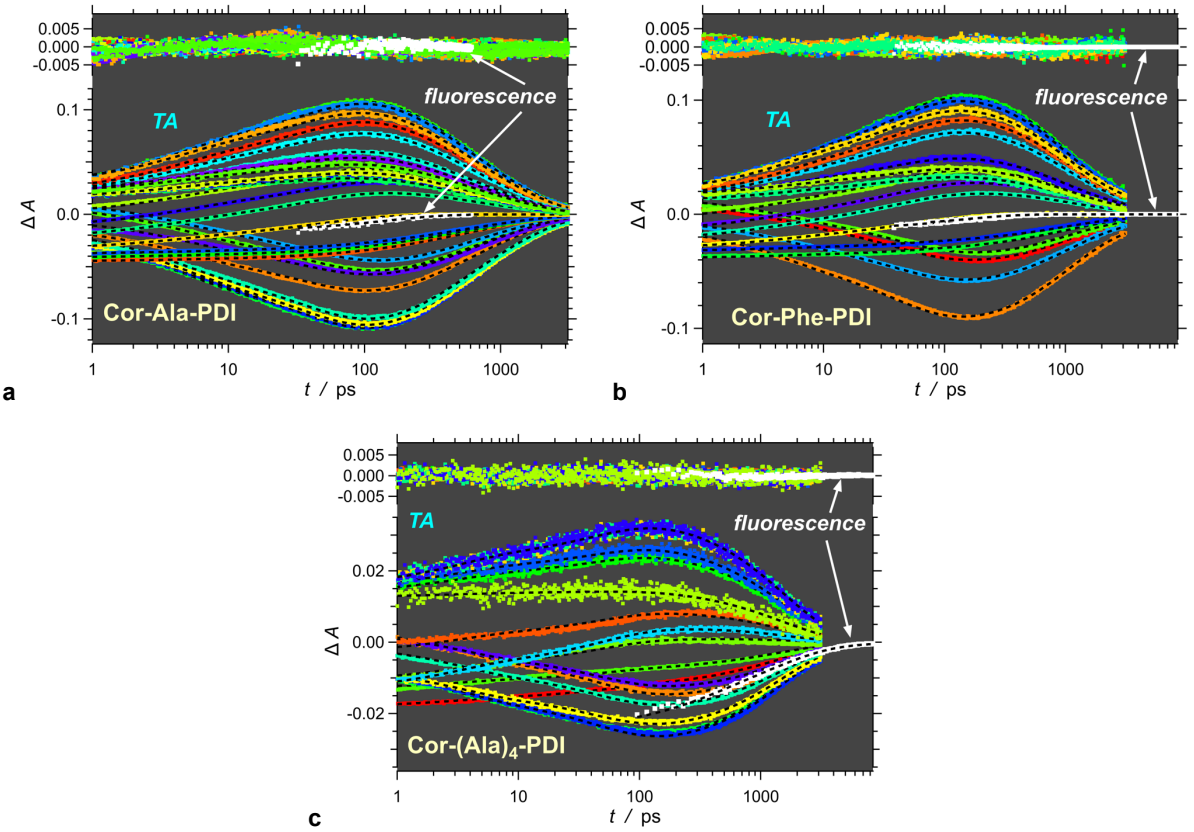


Figure S3. Global-fit analysis (using eq. 1 and 2) of TA and fluorescence-decay dynamics for the three conjugates (λ_{ex} = 400 nm). The fluorescence decays of ^{1}Cor* (λ_{fl} = 650 nm) are displayed in white. The TA traces for different wavelengths, recorded between 490 and 800 nm, are shown in different colors. The black dashed lines represent the global fits. The residuals from the data fits are on top of the graphs.

Excitation of the acceptor at 465 nm leads to different dynamics in the picosecond time domain involving an initial fast decrease followed by an increase in the amplitude in the NIR spectral region, for example, which is consistent with the decays of ^{1}PDI* to its ground state, followed by the growth of PDI$^{\bullet-}$ (Figure 7d,h). The locally excited, LE, state of the electron acceptor, ^{1}PDI*, in the DBA conjugates has five principal pathways for deactivation: (i) radiative decay to ground state, i.e., via fluorescence; (ii) non-radiative direct decays to ground state via internal conversion, i.e., ^{1}PDI* → ^{1}PDI; (iii) triplet formation via intersystem crossing; (iv) hole transfer, HT, to the electron donor, i.e., Cor–^{1}PDI* → Cor$^{\bullet+}$ --- PDI$^{\bullet-}$; and (v) resonance energy transfer, EnT, to the electron donor, i.e., Cor---^{1}PDI* → ^{1}Cor*---PDI. The first three pathways are inherent for PDI and are described by a single rate constant, $k_0^{(PDI)}$, determined from the excited-state lifetime of the chromophore in the absence of the electron donor, i.e., obtained from the optical emission decay of PDI (Figure S2b).

Because R_0 for EnT from PDI to Cor is 46 Å, which considerably exceeds the largest possible donor-acceptor distances in these DBA conjugates, it is reasonable to assume that it will dominate the excited state dynamics of PDI. Nevertheless, this estimate of R_0 assumes randomized orientation between the transition-dipole moments of Cor photoemission and PDI absorption. Conformers that lock orthogonal and close to orthogonal orientations between the transition dipole moments can suppress and even completely prevent EnT.

This model represented by eq. 1 and 2 leads to good global fits for the TA dynamics of the three DBA conjugates (Figure S4). For **Cor-(Ala)$_4$-PDI**, we also incorporated the fluorescence decay recorded at 560 nm, corresponding to the PDI emission (Figure S4c).

For the conjugates with short linkers, **Cor-Ala-PDI** and **Cor-Phe-PDI**, two exponential components can describe the PDI decay (depicting EnT and HT), i.e., m = 2, eq. S2 (Table 1). Similar to the results from the TA with selective excitation of the election donor, three exponential terms describe the ^{1}Cor* decay dynamics, i.e., n = 3, and CR shows biexponential character, i.e., w = 2 (Table 1).

When exciting the electron acceptor in **Cor-(Ala)$_4$-PDI**, incorporating the fluorescence decay of PDI (monitored at 560 nm) along with the TA kinetics requires four exponential terms for describing the ^{1}PDI* dynamics, m = 4, eq. S2. The forth component, however, does not have significant contribution, i.e., $k_4^{(PDI)}$ = 2.9 (±0.3) ×10^8 s^{-1} and $\alpha_4^{(PDI)}$ = 2×10^{-4}. While this component is consistent with the long-lived PDI fluorescence of **Cor-(Ala)$_4$-PDI** (Figure S2f), it does not truly contribute to the TA dynamics (Table 1). Similar to the TA analysis with 400-nm excitation, five exponential terms can describe the ^{1}Cor* deactivation, h = 5 and n = 4, eq. S2 (Table 1). In this case, however, a monoexponential decay function can fit well the CR dynamics (Figure S4c, Table 1).

The absorption of the PDI transients, along with the PDI stimulated-emission, dominate the TA spectra of the three conjugates, which is another one of their characteristic. In the visible spectral region, the PDI transients have larger molar extinction coefficients than the Cor transients. PDI has considerably larger fluorescence quantum yields than Cor. Therefore, the absorption of the PDI transients, along with the PDI stimulated-emission, dominate the TA spectra of the three conjugates.

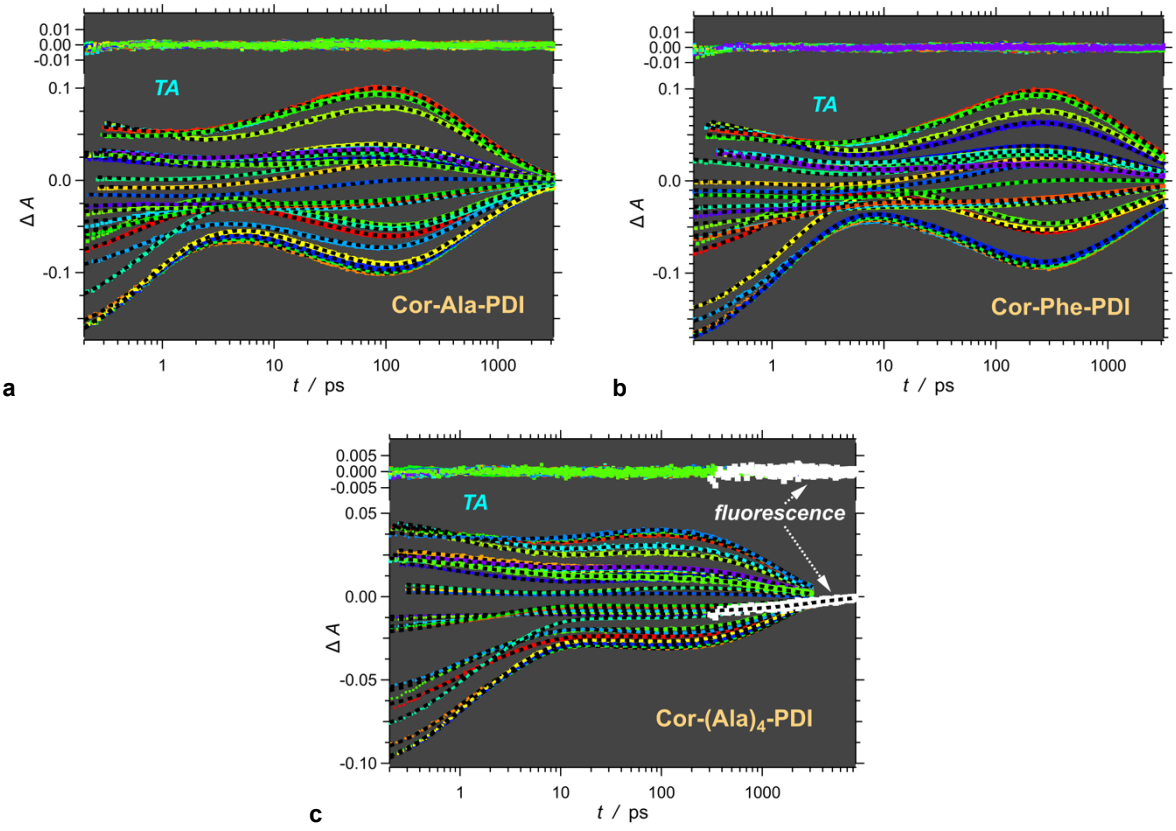


Figure S4. Global-fit analysis (using eq. 1 and 2) of TA dynamics for the three conjugates (λ_{ex} = 465 nm). (c) For **Cor-(Ala)$_4$-PDI**, we also incorporate the fluorescence decays of ^{1}PDI* (λ_{fl} = 560 nm), displayed in white, in the analysis. The TA traces for different wavelengths, recorded between 490 and 800 nm, are shown in different colors. The black dashed lines represent the global fits. The residuals from the data fits are on top of the graphs.

6. Computational analysis

All calculations were performed within the density functional theory (DFT) approach using Gaussian 09 program suite.[11] Geometry was optimized with the B3LYP functional, employing the 6-31G(d,p) basis set. Solvent effects were considered within the SCRF theory using the polarized continuum model (PCM) approach to model the interaction with the solvent. The structures were optimized in chloroform (for comparison with experimental NMR data) and in toluene (for comparison with ECD spectra). The results were highly similar. Excited electronic states were determined at the B3LYP/6-31G level by means of the time-dependent DFT (TD DFT) approach (100 excited states in each case). The ECD spectra were simulated by overlapping Gaussian functions for each transition where the width of the band at 1/e height is fixed at 0.1 eV. Aliphatic chains were shortened since their lengths have negligible influence on UV-VIS and ECD spectra.

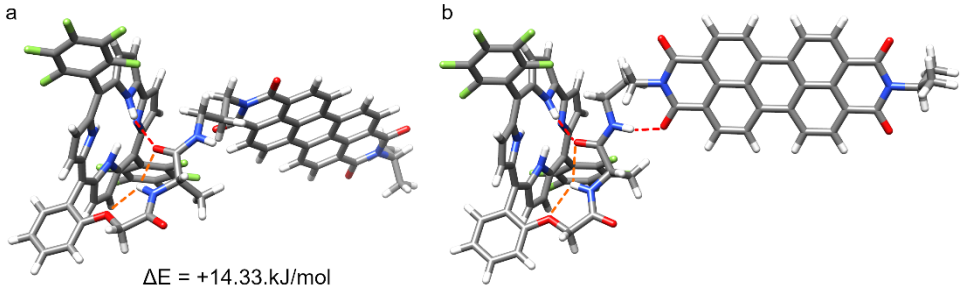


Figure S5. Structures of **Cor-Ala-PDI**$_{opt}$ obtained by geometry optimization (DFT 6-31G(d,p) in chloroform): (a) **Cor-Ala-PDI**$_{opt}$ without hydrogen bond to PDI; (b) **Cor-Ala-PDI**$_{opt}$ with hydrogen bond to PDI.

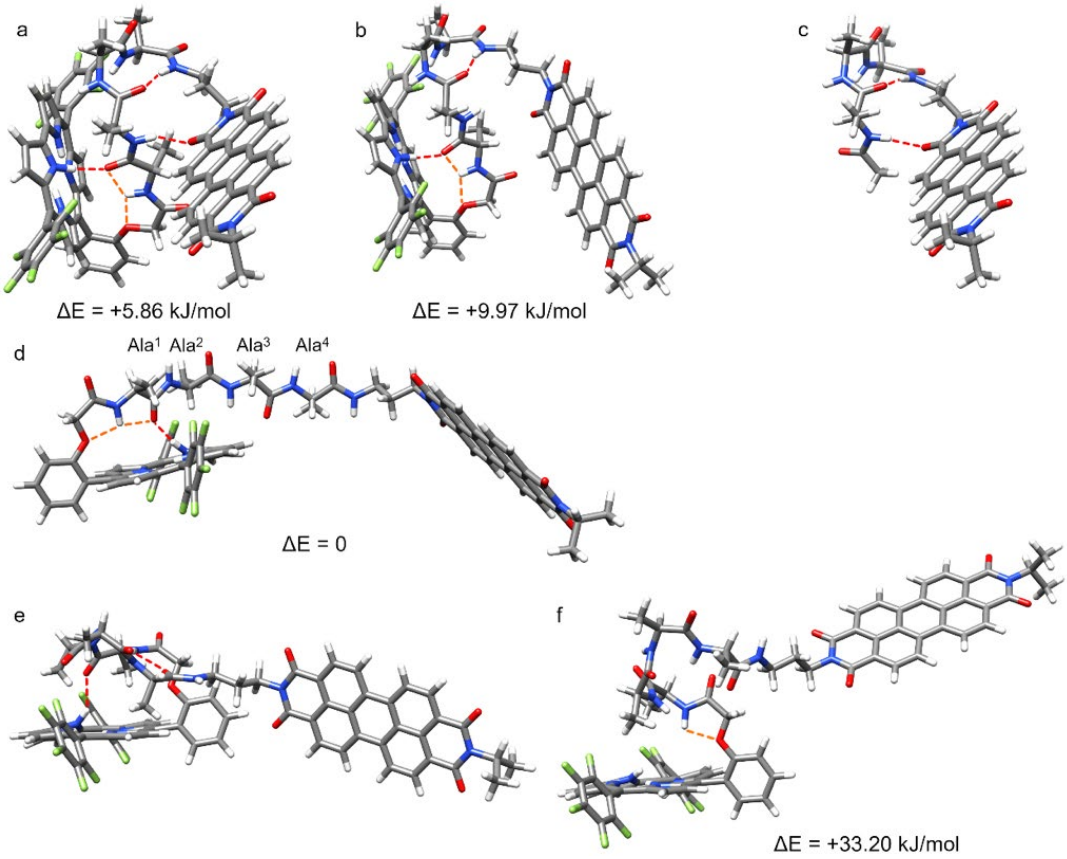


Figure S6. Structures of **Cor-(Ala)$_4$-PDI** obtained by geometry optimization (DFT 6-31G(d,p) in chloroform): (a) folded **Cor-(Ala)$_4$-PDI**$_{opt}$ with hydrogen bond to PDI; b) folded **Cor-(Ala)$_4$-PDI**$_{opt}$ without hydrogen bond to PDI; (c) folded **(Ala)$_4$-PDI**$_{opt}$ with hydrogen bond to PDI; (d) extended **Cor-(Ala)$_4$-PDI**$_{opt}$; (e) turn1,4-**Cor-(Ala)$_4$-PDI**$_{initial}$; (f) turn1,4-**Cor-(Ala)$_4$-PDI**$_{opt}$**.**

Atomic coordinates for all calculated geometries:

Cor-Ala-PDI$_{opt}$ with hydrogen bond to PDI in chloroform

Energy total = -4733.31253682 a.u.

Symbol	X	Y	Z
C	-4.1504230	-0.6287080	-3.2054660
C	-4.0679930	-1.6059240	-4.2662100
H	-3.7214050	-1.4309010	-5.2763670
C	-4.5197870	-2.7876220	-3.7312200
H	-4.6225580	-3.7357360	-4.2421750
C	-4.8895460	-2.5057050	-2.3543600
C	-5.5765940	-3.3114920	-1.4152720
C	-6.0684290	-2.7867420	-0.1959950
C	-6.7753340	-3.4097480	0.8775570
H	-7.0663300	-4.4494770	0.9143190
C	-7.0158250	-2.4542320	1.8406660
H	-7.5440960	-2.5908770	2.7725350
C	-6.4653910	-1.2063480	1.3964220
C	-6.4764020	0.0258560	2.0964600
C	-6.0312490	1.2765620	1.6344010
C	-5.8550690	2.4765260	2.4020420
H	-6.0823280	2.5631010	3.4539970
C	-5.3171030	3.4470340	1.5922280
H	-5.0275860	4.4455920	1.8858040
C	-5.1310660	2.8999600	0.2829510
C	-4.5589880	3.4928530	-0.8613800
C	-4.2021280	2.7243160	-2.0044900
C	-4.0946660	3.0387740	-3.3865580
H	-4.2074440	4.0263820	-3.8114750
C	-3.9463310	1.8435940	-4.0924710
H	-3.9212750	1.7313210	-5.1675230
C	-3.9575760	0.7814570	-3.1567320
N	-4.6189290	-1.1996980	-2.0742000
N	-5.9164030	-1.4600270	0.1611060
N	-5.5992480	1.5936480	0.3587870
N	-4.0669290	1.3603910	-1.9132420
H	-3.7577420	0.8789350	-1.0668750
C	-6.9270840	-0.0323040	3.5269930
C	-6.0185510	-0.4568030	4.5221940
C	-6.4061840	-0.5235480	5.8629170
H	-5.7107760	-0.8572640	6.6242400
C	-7.7072780	-0.1581800	6.2215710
H	-8.0029450	-0.2129410	7.2650480
C	-8.6154810	0.2713460	5.2567240
H	-9.6240600	0.5562370	5.5382320
C	-8.2176350	0.3315650	3.9174990
H	-8.9160760	0.6644300	3.1553520
O	-4.7699570	-0.7826230	4.0704180
C	-3.7201960	-1.0574930	4.9853250
H	-3.6300050	-0.2654840	5.7395400
H	-3.8787500	-2.0094930	5.5063060
C	-2.3913280	-1.1419970	4.2318900
O	-1.3660660	-1.4414090	4.8461010
N	-2.4444320	-0.8558190	2.9166510
H	-3.3295650	-0.6145590	2.4862140
C	-5.8266480	-4.7425110	-1.7303350
C	-4.7691700	-5.6387990	-1.9342940
C	-4.9790580	-6.9786890	-2.2465970
C	-6.2782860	-7.4640200	-2.3599520
C	-7.3540370	-6.6036630	-2.1628010
C	-7.1197290	-5.2657340	-1.8591940
F	-3.4997470	-5.2202910	-1.8180580
F	-3.9400990	-7.8052360	-2.4270010
F	-6.4917840	-8.7499880	-2.6568180

F	-8.6067620	-7.0636680	-2.2820670
F	-8.1887450	-4.4698660	-1.7008880
C	-4.3376650	4.9555830	-0.8924650
C	-3.0795600	5.4976760	-1.1992710
C	-2.8507290	6.8683800	-1.2564360
C	-3.8941220	7.7525180	-0.9975340
C	-5.1557910	7.2545250	-0.6862270
C	-5.3646910	5.8794860	-0.6443330
F	-2.0305650	4.6888590	-1.4284350
F	-1.6307280	7.3418990	-1.5421920
F	-3.6849380	9.0716640	-1.0459480
F	-6.1664410	8.1012140	-0.4497870
F	-6.6068910	5.4523340	-0.3713770
C	-1.2725410	-0.8640550	2.0596810
H	-0.4330650	-0.4451290	2.6243590
C	-0.9006690	-2.2874830	1.6004180
H	-1.7131010	-2.7231480	1.0119380
H	0.0075740	-2.2734390	0.9911730
C	-1.5807160	0.0286680	0.8469270
N	-0.5075630	0.5393170	0.2244240
H	0.4222390	0.3771750	0.6082870
O	-2.7510950	0.2093320	0.4761520
N	3.0540300	2.0317720	-0.4823120
N	13.8172330	-1.6478850	0.5101800
O	3.7275570	3.5920930	-2.0131020
O	2.3676980	0.4050270	0.9649250
O	14.4604320	-0.0651670	-1.0164570
O	13.0971330	-3.2176780	2.0249990
C	4.0344650	2.6741520	-1.2613110
C	5.4222090	2.1869260	-1.1165360
C	5.7280710	1.1110160	-0.2481850
C	4.6921330	0.4874520	0.4899500
C	3.2968530	0.9469590	0.3584570
C	4.9898620	-0.5675330	1.3378260
H	4.1874940	-1.0368320	1.8954710
C	6.3056250	-1.0190460	1.4725300
H	6.4895900	-1.8444900	2.1480340
C	7.3595750	-0.4369180	0.7643430
C	7.0751880	0.6520530	-0.1202770
C	8.1046690	1.2925400	-0.8810010
C	7.7557240	2.3501290	-1.7240960
C	6.4352790	2.7923780	-1.8427500
H	6.1871890	3.6146780	-2.5042030
C	9.4897730	0.8174660	-0.7525170
C	10.5438140	1.3896720	-1.4677430
H	10.3613420	2.2123350	-2.1473640
C	11.8587380	0.9300790	-1.3384710
H	12.6612430	1.3887550	-1.9044990
C	12.1557040	-0.1189220	-0.4847070
C	11.1195810	-0.7287410	0.2598770
C	9.7732450	-0.2685500	0.1339850
C	8.7459640	-0.9071980	0.8972730
C	9.0984990	-1.9599590	1.7443530
C	10.4205030	-2.4018770	1.8616230
H	10.6703490	-3.2212040	2.5257260
C	11.4303710	-1.7992450	1.1299700
C	12.8225610	-2.2885170	1.2718560
C	13.5588040	-0.5874040	-0.3677580
C	1.6616610	2.5013140	-0.5890300
H	1.7071460	3.5292180	-0.9422430
C	0.8043940	1.6277670	-1.5367700
H	1.3092040	0.6721730	-1.7133840
H	0.7134210	2.1180220	-2.5099470
C	15.2199450	-2.1516860	0.6600560
H	15.1178580	-2.9494310	1.3944350
C	16.1497050	-1.0839620	1.2469390

H	15.7369620	-0.6772070	2.1753040
H	16.3182810	-0.2650230	0.5467430
C	15.7422120	-2.7700510	-0.6413840
H	15.8817470	-2.0177470	-1.4186960
H	15.0544830	-3.5374030	-1.0099410
H	8.5123040	2.8549440	-2.3110030
H	8.3444860	-2.4628690	2.3363990
C	-0.5968160	1.3494260	-0.9915070
H	17.1138710	-1.5454380	1.4828270
H	16.7059750	-3.2502760	-0.4445330
H	1.2514180	2.4991300	0.4220850
H	-1.1881810	0.8132130	-1.7398460
H	-1.1244060	2.2872410	-0.7783210
H	-5.7448700	1.0208460	-0.4576460
H	-0.7219010	-2.9120200	2.4784820
H	-5.3029470	-0.9036690	-0.4493020

Cor-Ala-PDI$_{opt}$ with hydrogen bond to PDI in toluene

Energy total = -4733.30472140 a.u.

Symbol	X	Y	Z
C	-4.1588920	-0.6198330	-3.2043410
C	-4.0740420	-1.5978500	-4.2644740
H	-3.7256350	-1.4237970	-5.2741520
C	-4.5253940	-2.7790240	-3.7294170
H	-4.6259290	-3.7277470	-4.2395410
C	-4.8976710	-2.4962450	-2.3532440
C	-5.5837100	-3.3024070	-1.4145450
C	-6.0752590	-2.7785140	-0.1946390
C	-6.7831700	-3.4013270	0.8780480
H	-7.0771830	-4.4402110	0.9129530
C	-7.0216340	-2.4465960	1.8422960
H	-7.5504670	-2.5825380	2.7739140
C	-6.4687490	-1.1996910	1.3991420
C	-6.4781110	0.0323670	2.0998260
C	-6.0326740	1.2828870	1.6384410
C	-5.8576040	2.4827800	2.4063940
H	-6.0877810	2.5690130	3.4577190
C	-5.3180590	3.4529090	1.5976890
H	-5.0297410	4.4517060	1.8914570
C	-5.1298370	2.9062470	0.2884990
C	-4.5550970	3.4992590	-0.8542380
C	-4.2010760	2.7318100	-1.9993840
C	-4.0939680	3.0479790	-3.3807210
H	-4.2048730	4.0364330	-3.8041340
C	-3.9497540	1.8533350	-4.0887330
H	-3.9271400	1.7429510	-5.1640340
C	-3.9633440	0.7899760	-3.1550150
N	-4.6291470	-1.1898140	-2.0740840
N	-5.9204630	-1.4529860	0.1638700
N	-5.5994700	1.6006350	0.3633520
N	-4.0699580	1.3674760	-1.9105160
H	-3.7583720	0.8838540	-1.0659680
C	-6.9262290	-0.0269290	3.5310450
C	-6.0166870	-0.4571630	4.5230200
C	-6.4012960	-0.5254330	5.8644910
H	-5.7048980	-0.8636240	6.6230180
C	-7.6999820	-0.1559220	6.2273140
H	-7.9933820	-0.2119290	7.2714180
C	-8.6087800	0.2792070	5.2659100
H	-9.6155780	0.5672360	5.5506470
C	-8.2141300	0.3408530	3.9258200
H	-8.9129970	0.6778970	3.1659130
O	-4.7710750	-0.7858800	4.0670620
C	-3.7193150	-1.0709120	4.9760300

H	-3.6215670	-0.2832370	5.7340370
H	-3.8807220	-2.0247020	5.4930930
C	-2.3931230	-1.1592430	4.2170590
O	-1.3680690	-1.4656300	4.8254340
N	-2.4512130	-0.8670740	2.9023230
H	-3.3363690	-0.6205360	2.4751380
C	-5.8318380	-4.7338020	-1.7294420
C	-4.7725310	-5.6281920	-1.9336680
C	-4.9803310	-6.9687180	-2.2458780
C	-6.2789840	-7.4563940	-2.3583970
C	-7.3563730	-6.5978920	-2.1605020
C	-7.1243630	-5.2591520	-1.8572600
F	-3.5042820	-5.2076180	-1.8181050
F	-3.9402900	-7.7933900	-2.4268010
F	-6.4903440	-8.7426060	-2.6549660
F	-8.6079860	-7.0603730	-2.2786090
F	-8.1941890	-4.4656080	-1.6978610
C	-4.3274320	4.9609380	-0.8824270
C	-3.0666480	5.4978700	-1.1882980
C	-2.8312980	6.8677400	-1.2439630
C	-3.8706880	7.7565710	-0.9837130
C	-5.1347720	7.2638690	-0.6726860
C	-5.3503190	5.8894580	-0.6328630
F	-2.0210850	4.6847290	-1.4177850
F	-1.6091950	7.3357480	-1.5287320
F	-3.6553850	9.0746080	-1.0302630
F	-6.1410090	8.1148490	-0.4347870
F	-6.5939350	5.4679230	-0.3602710
C	-1.2815770	-0.8782040	2.0431960
H	-0.4390640	-0.4644120	2.6075270
C	-0.9153830	-2.3022710	1.5809370
H	-1.7300880	-2.7339790	0.9926730
H	-0.0076930	-2.2905890	0.9705550
C	-1.5885070	0.0175520	0.8327390
N	-0.5133810	0.5223670	0.2066640
H	0.4161750	0.3546300	0.5879670
O	-2.7577800	0.2070250	0.4657260
N	3.0486670	2.0148970	-0.4989870
N	13.8186630	-1.6424720	0.5214260
O	3.7245090	3.5785120	-2.0261410
O	2.3625430	0.3827080	0.9425710
O	14.4611730	-0.0571990	-1.0035270
O	13.0966030	-3.2124640	2.0356360
C	4.0301790	2.6605510	-1.2756360
C	5.4187010	2.1744720	-1.1278440
C	5.7245430	1.0984160	-0.2597710
C	4.6876590	0.4721230	0.4747050
C	3.2910850	0.9286660	0.3399450
C	4.9847230	-0.5828930	1.3224620
H	4.1804260	-1.0532460	1.8766430
C	6.3012110	-1.0314160	1.4606960
H	6.4853530	-1.8572380	2.1359040
C	7.3564910	-0.4466510	0.7566860
C	7.0723520	0.6421990	-0.1283140
C	8.1025460	1.2852920	-0.8860140
C	7.7529640	2.3424770	-1.7293340
C	6.4320120	2.7825240	-1.8511260
H	6.1818900	3.6048040	-2.5120160
C	9.4883350	0.8130550	-0.7539160
C	10.5435820	1.3870230	-1.4658510
H	10.3608000	2.2094550	-2.1459180
C	11.8593680	0.9304900	-1.3329920
H	12.6640920	1.3894520	-1.8958330
C	12.1556520	-0.1174910	-0.4782380
C	11.1186440	-0.7292830	0.2633830
C	9.7715450	-0.2723000	0.1334660

C	8.7437250	-0.9133330	0.8940270
C	9.0971670	-1.9645070	1.7426050
C	10.4199700	-2.4033850	1.8640340
H	10.6722230	-3.2215250	2.5288560
C	11.4297970	-1.7985860	1.1347080
C	12.8235170	-2.2852560	1.2812960
C	13.5606820	-0.5824270	-0.3573890
C	1.6561980	2.4842400	-0.6068490
H	1.7026850	3.5119620	-0.9608960
C	0.7982200	1.6111060	-1.5543530
H	1.3025470	0.6550650	-1.7307240
H	0.7079610	2.1015840	-2.5275420
C	15.2221380	-2.1430870	0.6752720
H	15.1194870	-2.9418270	1.4087110
C	16.1468420	-1.0723310	1.2647040
H	15.7318290	-0.6690460	2.1936040
H	16.3123690	-0.2517670	0.5656620
C	15.7496650	-2.7574450	-0.6259670
H	15.8873990	-2.0032740	-1.4017810
H	15.0663320	-3.5277130	-0.9966940
H	8.5104990	2.8487980	-2.3139420
H	8.3423560	-2.4684760	2.3329970
C	-0.6029280	1.3335250	-1.0081330
H	17.1128630	-1.5298270	1.5009640
H	16.7151210	-3.2339100	-0.4280230
H	1.2451630	2.4814370	0.4040770
H	-1.1959990	0.7992730	-1.7566500
H	-1.1295350	2.2718000	-0.7942030
H	-5.7373520	1.0252030	-0.4525120
H	-0.7375230	-2.9276180	2.4585750
H	-5.3052190	-0.8979220	-0.4461040

Cor-Ala-PDI$_{opt}$ without hydrogen bond to PDI in chloroform

Energy total = -4733.30707714 a.u.

Symbol	X	Y	Z
C	2.1715570	-0.4470080	-2.5244940
C	0.9660820	-0.2877750	-3.3036370
H	0.5493370	-1.0056010	-3.9979630
C	0.4670710	0.9497900	-2.9810310
H	-0.4202710	1.4187300	-3.3841740
C	1.3913080	1.5362060	-2.0261370
C	1.4399550	2.8526860	-1.5069660
C	2.5587870	3.3300170	-0.7838320
C	2.8124370	4.5925370	-0.1659740
H	2.1360790	5.4349340	-0.1652450
C	4.0573290	4.5372890	0.4215470
H	4.5538780	5.3288400	0.9621940
C	4.6202580	3.2376480	0.1851710
C	5.8748390	2.7537840	0.6318810
C	6.4551540	1.5005940	0.3639100
C	7.6442160	0.9501620	0.9458260
H	8.2658750	1.4642470	1.6631190
C	7.8217680	-0.3279540	0.4740470
H	8.6024620	-1.0177140	0.7599450
C	6.7577100	-0.6349680	-0.4293660
C	6.5005480	-1.8278260	-1.1352440
C	5.2713990	-2.0468140	-1.8140870
C	4.9266540	-2.8317840	-2.9486280
H	5.5894980	-3.5220970	-3.4510750
C	3.6484290	-2.4586500	-3.3640030
H	3.1327100	-2.8069500	-4.2480210
C	3.1864880	-1.4435030	-2.4919910
N	2.3909980	0.6482780	-1.7629720
N	3.6798290	2.5555660	-0.5524060

N	5.9603690	0.5066180	-0.4658490
N	4.1696490	-1.2711170	-1.5448730
H	3.9816570	-0.8250870	-0.6504610
C	6.6469860	3.6508160	1.5554460
C	6.6206390	3.4142350	2.9474820
C	7.3439360	4.2276180	3.8243450
H	7.3268120	4.0432230	4.8919660
C	8.0910600	5.2945540	3.3169440
H	8.6481510	5.9240060	4.0044050
C	8.1236420	5.5493920	1.9481090
H	8.7062680	6.3765340	1.5556680
C	7.4050280	4.7233050	1.0790130
H	7.4317680	4.9047510	0.0086080
O	5.8523220	2.3550860	3.3484510
C	5.8768800	1.9337680	4.7030680
H	6.8925120	1.6669100	5.0205780
H	5.5051210	2.7173970	5.3751530
C	4.9792220	0.7112290	4.8870540
O	4.8866940	0.1982460	6.0037620
N	4.3239350	0.2808410	3.7908130
H	4.4596860	0.7401720	2.8973520
C	0.2936710	3.7672730	-1.7526380
C	-0.9938490	3.4554510	-1.2946970
C	-2.0928440	4.2704660	-1.5453040
C	-1.9266820	5.4524160	-2.2599340
C	-0.6606430	5.8019800	-2.7210770
C	0.4219720	4.9628900	-2.4713980
F	-1.2046150	2.3410920	-0.5811970
F	-3.3075150	3.9243410	-1.0903550
F	-2.9743640	6.2468500	-2.5021610
F	-0.4946260	6.9338680	-3.4186410
F	1.6159400	5.3303010	-2.9619460
C	7.5506220	-2.8682890	-1.2179530
C	7.2874120	-4.2005360	-0.8619140
C	8.2499140	-5.2007800	-0.9519350
C	9.5286780	-4.8887040	-1.4039510
C	9.8290000	-3.5789850	-1.7658580
C	8.8481290	-2.5958830	-1.6786850
F	6.0782500	-4.5469050	-0.3948680
F	7.9585690	-6.4574340	-0.5904450
F	10.4626380	-5.8408830	-1.4893030
F	11.0536140	-3.2763560	-2.2167100
F	9.1806650	-1.3572780	-2.0731400
C	3.3667900	-0.8085760	3.8388060
H	3.8119410	-1.6408620	4.3973360
C	2.0613040	-0.3815240	4.5419610
H	1.5766470	0.4265000	3.9865050
H	1.3602730	-1.2163730	4.6253290
C	3.0846830	-1.2589030	2.3940670
N	2.3828850	-2.4121280	2.2936800
H	2.1282630	-2.8800680	3.1529680
O	3.4500330	-0.5817340	1.4277990
N	-1.9790540	-2.7103180	-0.0455530
N	-13.1220230	-0.2479340	0.4488340
O	-1.5109280	-0.5020230	-0.3660980
O	-2.4510970	-4.9109020	0.3625330
O	-12.6079810	1.9687520	0.1800860
O	-13.5629370	-2.4854010	0.7277650
C	-2.3603090	-1.3672580	-0.1924980
C	-3.8057290	-1.0618050	-0.1253510
C	-4.7510140	-2.0932980	0.0903750
C	-4.3072360	-3.4296790	0.2487720
C	-2.8645930	-3.7664650	0.2001590
C	-5.2331560	-4.4381050	0.4574120
H	-4.8804650	-5.4559110	0.5793910
C	-6.6005410	-4.1485300	0.5081030

H	-7.2853680	-4.9708960	0.6712470
C	-7.0836230	-2.8469530	0.3587830
C	-6.1452780	-1.7863820	0.1515580
C	-6.5655880	-0.4261730	0.0039080
C	-5.5957660	0.5561200	-0.2085350
C	-4.2330780	0.2479150	-0.2737420
H	-3.4997570	1.0297310	-0.4384520
C	-7.9990710	-0.1090420	0.0814850
C	-8.4810200	1.1970780	-0.0271700
H	-7.7953300	2.0231560	-0.1661040
C	-9.8476340	1.4874800	0.0396340
H	-10.1990020	2.5092210	-0.0471600
C	-10.7743680	0.4734170	0.2158370
C	-10.3316460	-0.8643270	0.3349820
C	-8.9376670	-1.1714870	0.2742040
C	-8.5190830	-2.5328410	0.4080150
C	-9.4932850	-3.5182690	0.5824030
C	-10.8558660	-3.2073560	0.6346180
H	-11.5946040	-3.9888470	0.7701860
C	-11.2829790	-1.8950650	0.5149260
C	-12.7324450	-1.5943610	0.5748760
C	-12.2177780	0.8087310	0.2774870
C	-0.5351690	-3.0017020	-0.1214530
H	-0.1293520	-2.4039570	-0.9398130
C	0.1874060	-2.6606460	1.1869420
H	-0.2120270	-3.2838220	1.9965490
H	-0.0109490	-1.6151330	1.4386230
C	-14.5898870	0.0437460	0.5038000
H	-15.0321190	-0.9427450	0.6355510
C	-15.1031720	0.6211350	-0.8199020
H	-14.8305440	-0.0278980	-1.6577920
H	-14.7079300	1.6207760	-1.0041690
C	-14.9553860	0.8938830	1.7254760
H	-14.5545640	1.9051650	1.6475920
H	-14.5802960	0.4334940	2.6447090
H	-5.8830720	1.5928610	-0.3305780
H	-9.2086550	-4.5582250	0.6807030
C	1.7063300	-2.8551050	1.0772090
H	-16.1956300	0.6791610	-0.7821900
H	-16.0456590	0.9554210	1.8019430
H	-0.4396800	-4.0600690	-0.3621490
H	2.1085540	-2.2631960	0.2541660
H	1.9562820	-3.9049900	0.8885420
H	2.2997220	-0.0309080	5.5475500
H	5.2853430	0.6645810	-1.1982040
H	3.5910280	1.5645350	-0.8130500

Cor-Ala-PDI$_{opt}$ without hydrogen bond to PDI in toluene

Energy total = -4733.29869576 a.u.

Symbol	X	Y	Z
C	2.6808860	-0.7866350	-2.5300080
C	1.4444940	-0.7234430	-3.2726980
H	1.0498710	-1.4856430	-3.9318080
C	0.8760900	0.4900490	-2.9650520
H	-0.0626150	0.8812750	-3.3315150
C	1.7919620	1.1583460	-2.0573390
C	1.7664550	2.4792770	-1.5525960
C	2.8571850	3.0408710	-0.8536580
C	3.0414400	4.3365450	-0.2811260
H	2.3213590	5.1415880	-0.3167510
C	4.2848830	4.3666370	0.3120580
H	4.7387900	5.2010150	0.8253540
C	4.9133830	3.0883920	0.1265100
C	6.1793510	2.6741300	0.6099700

C	6.8105500	1.4349310	0.4008220
C	7.9996400	0.9482570	1.0369910
H	8.5795790	1.5101390	1.7533060
C	8.2344990	-0.3386570	0.6191400
H	9.0284320	-0.9904180	0.9533000
C	7.2100570	-0.7162420	-0.3032810
C	7.0165880	-1.9428140	-0.9686830
C	5.8191170	-2.2327890	-1.6778790
C	5.5384390	-3.0783520	-2.7857500
H	6.2407060	-3.7657040	-3.2359330
C	4.2606130	-2.7725590	-3.2555280
H	3.7851670	-3.1798270	-4.1368450
C	3.7363710	-1.7383750	-2.4450890
N	2.8555710	0.3434020	-1.8091410
N	4.0166460	2.3364080	-0.5945460
N	6.3742650	0.3944110	-0.4050690
N	4.6827320	-1.4872220	-1.4792440
H	4.4468010	-0.9955060	-0.6221070
C	6.8893740	3.6266550	1.5279110
C	6.8017840	3.4422540	2.9256360
C	7.4636710	4.3049210	3.8034260
H	7.4057690	4.1562870	4.8752930
C	8.2081700	5.3708880	3.2897740
H	8.7182430	6.0390750	3.9772660
C	8.3000050	5.5748350	1.9154070
H	8.8808010	6.4015010	1.5192450
C	7.6439660	4.6982730	1.0458640
H	7.7164080	4.8400700	-0.0284230
O	6.0455940	2.3753420	3.3255770
C	5.8883890	2.0818760	4.7040700
H	6.8368200	1.7755470	5.1617170
H	5.5069410	2.9500470	5.2570820
C	4.8786000	0.9471330	4.8820120
O	4.6893060	0.4832820	6.0064910
N	4.2225830	0.5625570	3.7680150
H	4.5120980	0.9141410	2.8622160
C	0.5479320	3.3035830	-1.7809610
C	-0.6489370	3.0126180	-1.1154460
C	-1.8237780	3.7121240	-1.3742630
C	-1.8166730	4.7524120	-2.2988300
C	-0.6367300	5.0853830	-2.9581280
C	0.5226050	4.3596310	-2.6974020
F	-0.6827630	2.0471530	-0.1885720
F	-2.9630700	3.3973390	-0.7384550
F	-2.9401430	5.4339880	-2.5486740
F	-0.6284990	6.0868400	-3.8479910
F	1.6347650	4.6912490	-3.3692690
C	8.1030730	-2.9489820	-0.9726580
C	7.8728230	-4.2729820	-0.5659550
C	8.8714430	-5.2417520	-0.5819590
C	10.1531480	-4.9044690	-1.0076530
C	10.4210750	-3.6015950	-1.4175280
C	9.4048690	-2.6507520	-1.4047240
F	6.6620870	-4.6403050	-0.1218490
F	8.6116810	-6.4908500	-0.1748980
F	11.1206820	-5.8259240	-1.0219330
F	11.6486090	-3.2756840	-1.8424490
F	9.7075680	-1.4195210	-1.8422750
C	3.1917900	-0.4606520	3.7784670
H	3.5854880	-1.3549820	4.2819840
C	1.9418100	0.0176870	4.5408170
H	1.4613770	0.8492330	4.0176530
H	1.2089380	-0.7840860	4.6734830
C	2.9079230	-0.8326290	2.3044020
N	1.8202030	-1.6105710	2.1117770
H	1.2978630	-1.9018110	2.9252350

O	3.6377770	-0.4291470	1.3937360
N	-2.4018590	-1.9218390	-0.4173330
N	-13.6913210	-0.5191570	0.6417640
O	-2.2657800	0.0893220	-1.5009580
O	-2.5596280	-3.9311370	0.6575000
O	-13.4923910	1.5339480	-0.3567270
O	-13.8147680	-2.5910490	1.6276880
C	-2.9636520	-0.7441710	-0.9360590
C	-4.4240860	-0.5660800	-0.7622180
C	-5.2153620	-1.5794830	-0.1692040
C	-4.5975850	-2.7634160	0.3012650
C	-3.1307030	-2.9419030	0.2088060
C	-5.3687100	-3.7568570	0.8808030
H	-4.8796980	-4.6554590	1.2396740
C	-6.7526820	-3.5992760	1.0042690
H	-7.3144030	-4.4034150	1.4626570
C	-7.4046670	-2.4451430	0.5648270
C	-6.6271200	-1.4037830	-0.0346350
C	-7.2244390	-0.1880250	-0.4967270
C	-6.4002450	0.7928010	-1.0521410
C	-5.0201480	0.6097670	-1.1866730
H	-4.3977890	1.3915200	-1.6058750
C	-8.6777600	-0.0097430	-0.3639340
C	-9.3322290	1.1427390	-0.8037920
H	-8.7727200	1.9458960	-1.2667160
C	-10.7152700	1.3041040	-0.6688720
H	-11.2036510	2.2071920	-1.0168050
C	-11.4851690	0.3108200	-0.0875250
C	-10.8658560	-0.8755080	0.3695920
C	-9.4543980	-1.0511480	0.2353560
C	-8.8570570	-2.2639010	0.7032420
C	-9.6793240	-3.2356070	1.2775680
C	-11.0599080	-3.0525330	1.4070850
H	-11.6797280	-3.8192730	1.8575820
C	-11.6587470	-1.8863090	0.9607120
C	-13.1240070	-1.7184690	1.1120780
C	-12.9501850	0.5086850	0.0432700
C	-0.9382010	-2.0924540	-0.4984100
H	-0.5918510	-1.5290540	-1.3638210
C	-0.2466470	-1.6091800	0.7831330
H	-0.7362000	-2.0892250	1.6393240
H	-0.3779620	-0.5268860	0.8837000
C	-15.1716990	-0.3591220	0.7996060
H	-15.4691290	-1.2865640	1.2872670
C	-15.8819580	-0.2868750	-0.5565280
H	-15.6144990	-1.1452340	-1.1805940
H	-15.6361870	0.6304080	-1.0930170
C	-15.5209570	0.8028430	1.7361620
H	-15.2646790	1.7674150	1.2964920
H	-15.0004200	0.6997090	2.6932980
H	-6.8208920	1.7301260	-1.3939650
H	-9.2568680	-4.1644170	1.6398170
C	1.2504930	-1.9462770	0.8091090
H	-16.9640510	-0.3161820	-0.3933260
H	-16.5969700	0.7856430	1.9368190
H	-0.7507800	-3.1559860	-0.6540700
H	1.8000160	-1.3751030	0.0595340
H	1.4032050	-3.0133560	0.6015030
H	2.2469230	0.3476320	5.5347860
H	5.7204290	0.5037160	-1.1651600
H	3.9878720	1.3368300	-0.8270710

Cor-Phe-PDI$_{opt}$ in chloroform

Energy total = -4964.36877585 a.u.

Symbol	X	Y	Z
C	-4.5655950	0.1064360	-3.4081390
C	-4.7068770	-0.7878710	-4.5340020
H	-4.4570610	-0.5695340	-5.5640700
C	-5.2179850	-1.9588120	-4.0290760
H	-5.4745260	-2.8505290	-4.5855750
C	-5.4000850	-1.7510560	-2.6024380
C	-6.0478070	-2.5619830	-1.6399790
C	-6.3363050	-2.0921820	-0.3358740
C	-6.9695280	-2.7303780	0.7743480
H	-7.3656690	-3.7354300	0.7749790
C	-6.9901370	-1.8372450	1.8239730
H	-7.4136820	-1.9984540	2.8041950
C	-6.3677480	-0.6163650	1.4004400
C	-6.1495980	0.5441130	2.1852450
C	-5.6158160	1.7743340	1.7623270
C	-5.1963300	2.8713880	2.5877550
H	-5.2798780	2.8886410	3.6639620
C	-4.6413040	3.8415210	1.7893310
H	-4.1933220	4.7683750	2.1171220
C	-4.6861930	3.3972070	0.4295080
C	-4.1810650	4.0197470	-0.7304510
C	-4.0614230	3.3233330	-1.9656470
C	-4.0777130	3.7469040	-3.3226350
H	-4.1131420	4.7751170	-3.6546620
C	-4.1650530	2.6109760	-4.1297320
H	-4.2792810	2.5941320	-5.2047510
C	-4.2006650	1.4775600	-3.2822320
N	-4.9667820	-0.5024550	-2.2708330
N	-6.0047120	-0.8191890	0.0888940
N	-5.3077720	2.1547520	0.4680950
N	-4.0902730	1.9508940	-1.9956350
H	-3.7456590	1.3614040	-1.2354200
C	-6.4162060	0.4080490	3.6562230
C	-5.4626950	-0.2378560	4.4753660
C	-5.6674460	-0.3644720	5.8512420
H	-4.9342570	-0.8627200	6.4750540
C	-6.8322900	0.1562680	6.4229440
H	-6.9877310	0.0541020	7.4928230
C	-7.7838070	0.7989330	5.6341060
H	-8.6863500	1.2031390	6.0809710
C	-7.5674550	0.9213430	4.2579930
H	-8.3002440	1.4236960	3.6333790
O	-4.3594530	-0.7100160	3.8215130
C	-3.2200340	-1.1608810	4.5383750
H	-2.9001150	-0.4242640	5.2849800
H	-3.4167490	-2.1097940	5.0527850
C	-2.0605380	-1.3790850	3.5622090
O	-0.9589860	-1.7107300	3.9958610
N	-2.3636170	-1.1870620	2.2590350
H	-3.2798400	-0.8236960	2.0253490
C	-6.4588380	-3.9411960	-2.0112990
C	-5.5114880	-4.9007710	-2.3918980
C	-5.8701990	-6.1934840	-2.7617850
C	-7.2114180	-6.5649470	-2.7532650
C	-8.1801510	-5.6395190	-2.3766930
C	-7.7982650	-4.3498800	-2.0184940
F	-4.2056600	-4.5926060	-2.3943240
F	-4.9338080	-7.0845130	-3.1135210
F	-7.5669320	-7.8052680	-3.1037150
F	-9.4734690	-5.9894960	-2.3761770
F	-8.7687800	-3.4856240	-1.6828190
C	-3.7704820	5.4405640	-0.6753190
C	-2.4892450	5.8444390	-1.0818220
C	-2.0832990	7.1744730	-1.0606660
C	-2.9651690	8.1564030	-0.6180900

C	-4.2435620	7.7955720	-0.2028340
C	-4.6316290	6.4598110	-0.2415520
F	-1.5891950	4.9310460	-1.4855780
F	-0.8462470	7.5129550	-1.4466510
F	-2.5854250	9.4375480	-0.5892930
F	-5.1003590	8.7381100	0.2114830
F	-5.8843480	6.1688740	0.1403380
C	-1.3955100	-1.2722560	1.1833480
H	-0.4022210	-1.3060790	1.6381090
C	-1.6074900	-2.5337080	0.2945090
H	-2.5863780	-2.4441170	-0.1881660
H	-0.8541220	-2.5068520	-0.5010390
C	-1.5658340	-0.0241730	0.3034830
N	-0.4436870	0.5089640	-0.2018390
H	0.4639220	0.1453520	0.0827770
O	-2.7044090	0.4065710	0.0655440
N	3.1687470	2.0709310	-0.1837670
N	13.9227030	-1.7572280	0.0699840
O	3.9072140	4.0960230	-0.9503370
O	2.4250750	0.0168890	0.4794940
O	14.6290650	0.2842360	-0.6937630
O	13.1410590	-3.7796500	0.8294480
C	4.1832110	2.9575250	-0.5902360
C	5.5687580	2.4440230	-0.5514530
C	5.8410630	1.1169960	-0.1393100
C	4.7733440	0.2637960	0.2330060
C	3.3796000	0.7451500	0.1921150
C	5.0383530	-1.0355980	0.6348650
H	4.2116910	-1.6778650	0.9160900
C	6.3523220	-1.5097900	0.6790630
H	6.5102250	-2.5308710	1.0015190
C	7.4371000	-0.7061370	0.3205390
C	7.1869380	0.6382430	-0.1026900
C	8.2492760	1.5154310	-0.4908670
C	7.9325870	2.8154960	-0.8913740
C	6.6132210	3.2757060	-0.9222430
H	6.3904000	4.2891840	-1.2359400
C	9.6334200	1.0214980	-0.4572230
C	10.7188600	1.8177090	-0.8285430
H	10.5628970	2.8372520	-1.1573650
C	12.0324630	1.3379900	-0.7927240
H	12.8598520	1.9735400	-1.0865310
C	12.2963410	0.0424980	-0.3809850
C	11.2278590	-0.7995530	0.0050190
C	9.8825820	-0.3205240	-0.0300040
C	8.8222920	-1.1965020	0.3626380
C	9.1423670	-2.4922850	0.7730800
C	10.4634560	-2.9510040	0.8054110
H	10.6880650	-3.9613240	1.1271520
C	11.5050240	-2.1208360	0.4256230
C	12.8954360	-2.6335770	0.4658380
C	13.6987950	-0.4412500	-0.3548110
C	1.7767090	2.5532220	-0.1854710
H	1.8243820	3.6390490	-0.1386770
C	0.9792570	2.0868390	-1.4261640
H	1.4898300	1.2394290	-1.8957850
H	0.9491170	2.8868350	-2.1710070
C	15.3232760	-2.2868490	0.1105490
H	15.1916340	-3.3053350	0.4731280
C	16.1876300	-1.5312310	1.1258560
H	15.7067460	-1.5157350	2.1087720
H	16.3791580	-0.5050490	0.8101580
C	15.9420900	-2.3583090	-1.2896980
H	16.1093520	-1.3650550	-1.7079560
H	15.2987000	-2.9254440	-1.9694450
H	8.7144790	3.5021990	-1.1893520

H	8.3626480	-3.1781010	1.0790860
C	-0.4536740	1.6739300	-1.0889250
H	17.1465160	-2.0488600	1.2297970
H	16.9038770	-2.8772220	-1.2271170
H	1.3159640	2.1844820	0.7323790
H	-0.9988200	1.4311990	-2.0073050
H	-0.9946440	2.4964150	-0.6075400
C	-1.5151120	-3.8376110	1.0537360
C	-0.2729140	-4.4415500	1.2937590
C	-2.6689350	-4.4643760	1.5433370
C	-0.1844130	-5.6381720	2.0051980
H	0.6321430	-3.9710110	0.9167730
C	-2.5845620	-5.6622240	2.2558650
H	-3.6398180	-4.0117160	1.3600350
C	-1.3414940	-6.2528330	2.4893340
H	0.7868770	-6.0927630	2.1784640
H	-3.4902390	-6.1354260	2.6247540
H	-1.2743660	-7.1861970	3.0406760
H	-5.6189990	1.6769710	-0.3628170
H	-5.4155900	-0.2767250	-0.5575320

Cor-Phe-PDI$_{opt}$ in toluene

Energy total = -4964.36035494 a.u.

Symbol	X	Y	Z
C	-4.3376990	0.0055280	-3.4097330
C	-4.3132000	-0.9205090	-4.5189160
H	-4.0065740	-0.7015480	-5.5333750
C	-4.7529160	-2.1229040	-4.0215370
H	-4.8847180	-3.0458770	-4.5706070
C	-5.0602690	-1.9034500	-2.6182490
C	-5.6999850	-2.7493870	-1.6829040
C	-6.1212080	-2.2843780	-0.4141860
C	-6.7844150	-2.9542890	0.6587610
H	-7.1068150	-3.9853840	0.6475280
C	-6.9441040	-2.0529000	1.6892290
H	-7.4228930	-2.2328990	2.6402880
C	-6.3821640	-0.7958070	1.2901040
C	-6.2925470	0.3842870	2.0720740
C	-5.8323880	1.6473620	1.6612980
C	-5.5402810	2.7806540	2.4930560
H	-5.6811120	2.7999190	3.5631750
C	-5.0198860	3.7827800	1.7119220
H	-4.6605080	4.7438720	2.0498260
C	-4.9584190	3.3240580	0.3573200
C	-4.4322390	3.9699800	-0.7796830
C	-4.1888010	3.2715630	-1.9962340
C	-4.1461230	3.6764200	-3.3578030
H	-4.2369500	4.6947700	-3.7091660
C	-4.0908060	2.5272660	-4.1497630
H	-4.1300820	2.4893170	-5.2295820
C	-4.0969930	1.4048610	-3.2878650
N	-4.7681150	-0.6137420	-2.2902080
N	-5.9172600	-0.9848830	0.0097170
N	-5.4883670	2.0394400	0.3794990
N	-4.1132140	1.9012210	-2.0052520
H	-3.7751760	1.3490440	-1.2143290
C	-6.6106560	0.2338680	3.5306150
C	-5.6647330	-0.3831490	4.3814090
C	-5.9152680	-0.5243890	5.7481520
H	-5.1885010	-1.0013740	6.3957000
C	-7.1165920	-0.0458130	6.2796890
H	-7.3070580	-0.1590620	7.3428300
C	-8.0599630	0.5691320	5.4599990
H	-8.9911280	0.9403520	5.8757440

C	-7.7991650	0.7049710	4.0928960
H	-8.5261240	1.1842070	3.4438040
O	-4.5222620	-0.8103550	3.7670340
C	-3.3955070	-1.2304990	4.5214970
H	-3.1367720	-0.4983210	5.2957140
H	-3.5748550	-2.1976130	5.0080290
C	-2.1858870	-1.3780870	3.5927910
O	-1.0888360	-1.6541880	4.0706150
N	-2.4442910	-1.1907740	2.2779050
H	-3.3631480	-0.8603180	2.0091280
C	-5.9463150	-4.1719910	-2.0381930
C	-4.8797070	-5.0528920	-2.2583780
C	-5.0776810	-6.3865770	-2.6045530
C	-6.3739810	-6.8772240	-2.7346420
C	-7.4580330	-6.0316460	-2.5169560
C	-7.2352490	-4.6996480	-2.1785500
F	-3.6160340	-4.6251430	-2.1162540
F	-4.0336180	-7.2015330	-2.8015750
F	-6.5770140	-8.1566620	-3.0644780
F	-8.7060250	-6.5002850	-2.6477830
F	-8.3075740	-3.9155390	-1.9928010
C	-4.1198750	5.4150760	-0.7181750
C	-2.8446190	5.8978380	-1.0522140
C	-2.5274800	7.2518500	-1.0239700
C	-3.4962440	8.1779140	-0.6465740
C	-4.7714300	7.7382500	-0.3026960
C	-5.0696400	6.3794860	-0.3478910
F	-1.8649240	5.0414460	-1.3892370
F	-1.2940950	7.6674440	-1.3392570
F	-3.2025860	9.4810810	-0.6115430
F	-5.7093700	8.6267740	0.0494280
F	-6.3206160	6.0103010	-0.0360170
C	-1.4193700	-1.1865690	1.2533160
H	-0.4514150	-1.1713980	1.7615170
C	-1.4996210	-2.4310380	0.3206750
H	-2.4465540	-2.3868790	-0.2271390
H	-0.6982320	-2.3363960	-0.4217660
C	-1.6172010	0.0726420	0.3949380
N	-0.5026790	0.6422820	-0.0899670
H	0.4100380	0.2959320	0.1995800
O	-2.7628870	0.4773110	0.1483940
N	3.0957210	2.2263980	-0.0964160
N	13.8677750	-1.5595440	0.1063080
O	3.8210520	4.2461310	-0.8902610
O	2.3662930	0.1737030	0.5877180
O	14.5576080	0.4739770	-0.6942090
O	13.0991540	-3.5738880	0.9007740
C	4.1036910	3.1131440	-0.5217170
C	5.4916220	2.6038270	-0.4907330
C	5.7726470	1.2823510	-0.0670620
C	4.7111470	0.4294490	0.3233240
C	3.3144690	0.9045060	0.2880780
C	4.9841790	-0.8642660	0.7372580
H	4.1611450	-1.5052480	1.0320260
C	6.3004050	-1.3327300	0.7761810
H	6.4651760	-2.3496340	1.1087060
C	7.3795330	-0.5296080	0.3998730
C	7.1206490	0.8088320	-0.0369870
C	8.1762040	1.6853190	-0.4450840
C	7.8504070	2.9796560	-0.8566510
C	6.5292350	3.4352800	-0.8800240
H	6.2978440	4.4443900	-1.2018850
C	9.5623640	1.1963510	-0.4192730
C	10.6417840	1.9904280	-0.8119710
H	10.4787540	3.0049090	-1.1533290
C	11.9576100	1.5159130	-0.7824960

H	12.7813870	2.1485210	-1.0927240
C	12.2295670	0.2274540	-0.3552960
C	11.1676610	-0.6127100	0.0521850
C	9.8202830	-0.1390660	0.0231440
C	8.7670580	-1.0139020	0.4367840
C	9.0966440	-2.3024640	0.8619480
C	10.4198260	-2.7559330	0.8888500
H	10.6535690	-3.7605470	1.2220960
C	11.4540540	-1.9268930	0.4882930
C	12.8475180	-2.4347040	0.5235000
C	13.6352030	-0.2506260	-0.3357510
C	1.7024410	2.7055330	-0.0901440
H	1.7492550	3.7917760	-0.0486440
C	0.8964550	2.2330780	-1.3232970
H	1.4091270	1.3888820	-1.7967380
H	0.8551940	3.0326310	-2.0681420
C	15.2707050	-2.0834230	0.1418250
H	15.1459880	-3.0969210	0.5208990
C	16.1412450	-1.3079540	1.1367180
H	15.6706950	-1.2804160	2.1243950
H	16.3240270	-0.2857800	0.8032720
C	15.8764970	-2.1719440	-1.2631720
H	16.0339790	-1.1838380	-1.6971400
H	15.2302740	-2.7530670	-1.9283060
H	8.6274020	3.6656080	-1.1692660
H	8.3221310	-2.9867730	1.1845980
C	-0.5305840	1.8084110	-0.9745960
H	17.1039540	-1.8189090	1.2388550
H	16.8418610	-2.6844970	-1.2025180
H	1.2491040	2.3390920	0.8324010
H	-1.0799260	1.5610380	-1.8890760
H	-1.0761870	2.6269200	-0.4906080
C	-1.3797930	-3.7510770	1.0477840
C	-0.1327030	-4.2222630	1.4811940
C	-2.5150970	-4.5291480	1.3067350
C	-0.0225770	-5.4371790	2.1564220
H	0.7594380	-3.6316110	1.2866950
C	-2.4090060	-5.7467090	1.9821750
H	-3.4877960	-4.1783950	0.9726880
C	-1.1620760	-6.2044380	2.4092140
H	0.9524680	-5.7867120	2.4838800
H	-3.3004290	-6.3382050	2.1716020
H	-1.0771130	-7.1522490	2.9328480
H	-5.7095830	1.5280580	-0.4601400
H	-5.3280800	-0.4054440	-0.6031630

Extended Cor-$(Ala)_4$-PDI_{opt} in chloroform

Energy total = -5475.33678397 a.u.

Symbol	X	Y	Z
O	-9.9498730	-3.1250660	0.8974320
C	-3.6599530	0.0696750	-0.5576640
C	-2.3109830	-0.2699100	-0.2586800
H	-1.4968860	0.4375900	-0.1907550
C	-2.2587730	-1.6461390	-0.0574450
H	-1.3769890	-2.2292540	0.1674910
C	-3.5765650	-2.1681840	-0.2387560
C	-4.1422090	-3.4652570	-0.2940560
C	-5.4907280	-3.6894110	-0.6657550
C	-6.1760140	-4.9690100	-0.6273460
H	-5.7335760	-5.9180070	-0.3578940
C	-7.4744460	-4.7290150	-0.9584150
H	-8.2792070	-5.4468840	-1.0294890
C	-7.5900740	-3.3000390	-1.2111800
C	-8.8140070	-2.6459370	-1.5271080

C	-8.9766290	-1.2802170	-1.8031100
C	-10.1945480	-0.5413220	-1.9907800
H	-11.1822090	-0.9774990	-1.9759040
C	-9.8799760	0.7845440	-2.1528760
H	-10.5739640	1.6029880	-2.2776890
C	-8.4545090	0.9332610	-2.0657120
C	-7.6888920	2.1159140	-2.0948960
C	-6.3122730	2.1379970	-1.7414440
C	-5.2464670	3.0183920	-2.0528460
H	-5.3352260	3.9225880	-2.6384780
C	-4.0576790	2.4586960	-1.5729530
H	-3.0579720	2.8463160	-1.7076030
C	-4.3769140	1.2287450	-0.9600940
N	-4.3737310	-1.0924180	-0.4984720
H	-5.3529580	-1.2781720	-0.7493070
N	-6.3760310	-2.7009230	-1.0481740
N	-7.9633720	-0.3492460	-1.8816840
N	-5.7527670	1.0812530	-1.0519980
H	-6.2789310	0.5893870	-0.3227980
C	-10.0727120	-3.4553340	-1.4234420
C	-10.6290970	-3.6924140	-0.1458800
C	-11.7962460	-4.4461710	-0.0016820
H	-12.2215330	-4.6275280	0.9785020
C	-12.4238160	-4.9648730	-1.1388210
H	-13.3309780	-5.5501220	-1.0211200
C	-11.8978670	-4.7337620	-2.4074950
H	-12.3883610	-5.1361790	-3.2879740
C	-10.7270790	-3.9798990	-2.5397100
H	-10.3041760	-3.7971590	-3.5232260
C	-3.2778220	-4.6150970	0.0793870
C	-2.7477690	-4.7332200	1.3705740
C	-1.9235840	-5.7910920	1.7420260
C	-1.6090790	-6.7768430	0.8110970
C	-2.1207770	-6.6942800	-0.4805770
C	-2.9375650	-5.6229570	-0.8309480
F	-3.0449440	-3.8162610	2.3058570
F	-1.4419340	-5.8728220	2.9894130
F	-0.8198780	-7.7990380	1.1568630
F	-1.8122140	-7.6364520	-1.3815940
F	-3.3932080	-5.5735110	-2.0914810
C	-8.3278070	3.3866850	-2.5085320
C	-8.2973100	4.5209090	-1.6826590
C	-8.8694490	5.7318610	-2.0582990
C	-9.5063480	5.8398310	-3.2913730
C	-9.5607090	4.7356520	-4.1367340
C	-8.9725030	3.5368230	-3.7451570
F	-7.7186040	4.4594270	-0.4719310
F	-8.8252560	6.7879180	-1.2353340
F	-10.0634740	6.9971100	-3.6609880
F	-10.1613810	4.8383450	-5.3295140
F	-9.0265790	2.5102580	-4.6070510
C	-10.3652050	-3.3469060	2.2353090
H	-10.3641910	-4.4155060	2.4832880
H	-11.3747200	-2.9554790	2.4141440
C	-9.4085920	-2.6386190	3.1961820
O	-9.5913610	-2.7337090	4.4106050
N	-8.4095560	-1.9373920	2.6234180
H	-8.3359160	-1.8920920	1.6136730
C	-7.4276880	-1.2007920	3.3971710
H	-7.9310630	-0.7923640	4.2799480
C	-6.9071320	-0.0529930	2.5193340
O	-7.0192150	-0.1022880	1.2863620
N	-6.3093260	0.9567220	3.1798790
H	-6.2109060	0.9196210	4.1876260
C	-5.6064280	2.0581730	2.5291570
H	-5.4292940	1.7643480	1.4952580

C	-4.2718600	2.2356650	3.2695440
O	-4.2307470	2.1908260	4.5025420
C	-6.4215790	3.3603330	2.5605130
H	-6.6305020	3.6539340	3.5929860
H	-5.8670440	4.1678820	2.0734500
N	-3.1999670	2.4610790	2.4842500
H	-3.2714320	2.4257900	1.4727080
C	-1.8554170	2.6688580	3.0015420
H	-1.9034390	3.3969900	3.8182960
C	-1.0235310	3.2365190	1.8408190
O	-1.3253900	3.0010250	0.6639830
C	-1.2291120	1.3627440	3.5275050
H	-1.1760810	0.6199300	2.7267310
N	0.0524190	3.9602470	2.1995300
H	0.2955940	4.1166570	3.1728230
C	1.0195170	4.4788820	1.2456010
C	0.5007650	5.7393950	0.5282220
H	0.3093130	6.5383990	1.2500580
H	-0.4292130	5.4992360	0.0092270
H	1.2239660	6.1010200	-0.2083580
C	-6.2624680	-2.0993300	3.8614370
H	-7.3659460	3.2237280	2.0284860
H	-1.8475320	0.9693230	4.3362710
H	-0.2211970	1.5426440	3.9121950
H	1.2236180	3.7026660	0.4990800
H	-6.6649500	-2.9218080	4.4569510
H	-5.7233880	-2.5122030	3.0038700
H	-5.5558820	-1.5386670	4.4803170
C	2.3010780	4.7754500	2.0476290
N	3.4097240	4.9909910	1.3041560
H	3.3382820	4.9205510	0.2985140
O	2.2765670	4.8300910	3.2794400
N	8.2443670	3.8478290	1.6069720
N	16.8158750	-2.8957360	-1.7822950
O	8.6031240	5.2059580	-0.1941680
O	7.8192570	2.4328900	3.3491640
O	17.2155640	-1.4517670	-3.5162380
O	16.3631860	-4.2927740	-0.0152750
C	8.9261500	4.2023040	0.4346080
C	10.0351840	3.3196230	0.0114230
C	10.3580490	2.1548970	0.7495820
C	9.6100760	1.8284570	1.9069860
C	8.4982610	2.6928850	2.3607840
C	9.9209200	0.6856830	2.6252500
H	9.3395330	0.4472830	3.5086370
C	10.9684350	-0.1462200	2.2180660
H	11.1732830	-1.0274540	2.8126840
C	11.7346510	0.1362330	1.0851770
C	11.4313670	1.3116570	0.3266900
C	12.1751440	1.6645300	-0.8442070
C	11.8188740	2.8211330	-1.5410960
C	10.7638520	3.6376310	-1.1227640
H	10.5042630	4.5308690	-1.6795240
C	13.2855280	0.8023070	-1.2735910
C	14.0630230	1.0912570	-2.3970310
H	13.8639960	1.9759030	-2.9887180
C	15.1171860	0.2636020	-2.7974040
H	15.7086290	0.5083550	-3.6721310
C	15.4221110	-0.8824140	-2.0821830
C	14.6612660	-1.2146240	-0.9375050
C	13.5853020	-0.3743340	-0.5172670
C	12.8377170	-0.7320250	0.6486660
C	13.1854660	-1.8979520	1.3341540
C	14.2383030	-2.7162170	0.9116420
H	14.4890610	-3.6174390	1.4591070
C	14.9773740	-2.3869990	-0.2126460

C	16.0878910	-3.2714630	-0.6377710
C	16.5459810	-1.7412300	-2.5287930
C	7.1564360	4.7329950	2.0562870
H	7.4328530	5.7467890	1.7644350
C	5.8026980	4.3484220	1.4485230
H	5.5313500	3.3369630	1.7674000
H	5.8918400	4.3430850	0.3558280
C	17.9385980	-3.7939920	-2.2011110
H	17.9067390	-4.5910450	-1.4596220
C	19.2969540	-3.0936700	-2.0863130
H	19.4375640	-2.6827120	-1.0818390
H	19.3981270	-2.2883780	-2.8149040
C	17.6853730	-4.4180750	-3.5778030
H	17.7270650	-3.6732000	-4.3732860
H	16.7096140	-4.9127170	-3.6061740
H	12.3599910	3.1122440	-2.4324150
H	12.6387900	-2.1968060	2.2195820
C	4.7083050	5.3327240	1.8746330
H	20.0908980	-3.8261190	-2.2633220
H	18.4512770	-5.1763120	-3.7693550
H	7.1193410	4.6665400	3.1438910
H	4.9812310	6.3522800	1.5737130
H	4.5796710	5.3298190	2.9588280
H	-6.9931750	-0.6223440	-1.8657790

Extended Cor-$(Ala)_4$-PDI_{opt} in toluene

Energy total = -5475.32586830 a.u.

Symbol	X	Y	Z
O	-9.8842970	-3.1950720	0.9015760
C	-3.6547710	0.0982410	-0.5472150
C	-2.3017870	-0.2225830	-0.2463240
H	-1.4976690	0.4964570	-0.1804760
C	-2.2317550	-1.5976720	-0.0426520
H	-1.3428190	-2.1692310	0.1836940
C	-3.5420190	-2.1373710	-0.2244940
C	-4.0903990	-3.4420180	-0.2792260
C	-5.4344930	-3.6845060	-0.6540830
C	-6.1022930	-4.9735880	-0.6186380
H	-5.6474320	-5.9168940	-0.3501370
C	-7.4025070	-4.7513700	-0.9529990
H	-8.1970480	-5.4800300	-1.0283550
C	-7.5368450	-3.3237200	-1.2048300
C	-8.7689290	-2.6867760	-1.5244140
C	-8.9495540	-1.3242160	-1.8035320
C	-10.1769450	-0.6022000	-1.9945080
H	-11.1583470	-1.0522110	-1.9801420
C	-9.8797530	0.7271300	-2.1585190
H	-10.5842150	1.5360420	-2.2862430
C	-8.4565340	0.8952940	-2.0690790
C	-7.7074940	2.0885050	-2.0966080
C	-6.3318740	2.1298510	-1.7400590
C	-5.2777540	3.0258470	-2.0454930
H	-5.3774000	3.9300070	-2.6294300
C	-4.0825620	2.4825650	-1.5618810
H	-3.0877890	2.8849190	-1.6898120
C	-4.3864070	1.2471200	-0.9528600
N	-4.3529580	-1.0729750	-0.4868280
H	-5.3295460	-1.2731110	-0.7379050
N	-6.3323270	-2.7081300	-1.0375490
N	-7.9488250	-0.3801410	-1.8828640
N	-5.7596670	1.0800490	-1.0507090
H	-6.2816480	0.5804190	-0.3237140
C	-10.0162530	-3.5131860	-1.4197270
C	-10.5617260	-3.7656110	-0.1402910

C	-11.7174490	-4.5362180	0.0060740
H	-12.1334300	-4.7296730	0.9880220
C	-12.3451860	-5.0557660	-1.1304650
H	-13.2435690	-5.6541840	-1.0111840
C	-11.8305250	-4.8091530	-2.4005900
H	-12.3210540	-5.2125380	-3.2806280
C	-10.6706310	-4.0390800	-2.5351190
H	-10.2557070	-3.8447070	-3.5197900
C	-3.2113230	-4.5792960	0.0980420
C	-2.6793540	-4.6851680	1.3897470
C	-1.8409940	-5.7307010	1.7653020
C	-1.5139170	-6.7162040	0.8381040
C	-2.0272020	-6.6456690	-0.4539020
C	-2.8581100	-5.5862980	-0.8087230
F	-2.9880630	-3.7686110	2.3212610
F	-1.3577000	-5.8009380	3.0124620
F	-0.7113150	-7.7263470	1.1877240
F	-1.7065280	-7.5872630	-1.3508040
F	-3.3144100	-5.5480710	-2.0686370
C	-8.3633210	3.3507400	-2.5093660
C	-8.3467910	4.4852200	-1.6829650
C	-8.9343130	5.6893060	-2.0578220
C	-9.5737130	5.7897330	-3.2905190
C	-9.6151490	4.6848770	-4.1361220
C	-9.0110870	3.4932110	-3.7456410
F	-7.7672000	4.4307590	-0.4725300
F	-8.9027890	6.7453210	-1.2346150
F	-10.1453820	6.9399370	-3.6593060
F	-10.2180040	4.7803970	-5.3280250
F	-9.0528140	2.4669470	-4.6077170
C	-10.2882130	-3.4264070	2.2408850
H	-10.2660080	-4.4952640	2.4874130
H	-11.3040220	-3.0542860	2.4258560
C	-9.3409550	-2.7005720	3.1986850
O	-9.5205000	-2.7942080	4.4123720
N	-8.3527240	-1.9858900	2.6212410
H	-8.2809120	-1.9388340	1.6113950
C	-7.3895980	-1.2262540	3.3950900
H	-7.9054350	-0.8272900	4.2752900
C	-6.8923790	-0.0691170	2.5164480
O	-7.0096100	-0.1168810	1.2845580
N	-6.3092590	0.9511060	3.1759400
H	-6.1943080	0.9110690	4.1819430
C	-5.6235640	2.0609950	2.5216350
H	-5.4446960	1.7684160	1.4875810
C	-4.2900480	2.2561660	3.2594260
O	-4.2437810	2.2010730	4.4909250
C	-6.4562990	3.3519910	2.5529630
H	-6.6651070	3.6450570	3.5856510
H	-5.9151520	4.1661830	2.0618470
N	-3.2244750	2.5083520	2.4718250
H	-3.2965740	2.4701410	1.4603990
C	-1.8813380	2.7246920	2.9882210
H	-1.9324640	3.4571830	3.8012970
C	-1.0511880	3.2891250	1.8250520
O	-1.3513710	3.0504540	0.6491420
C	-1.2486600	1.4249350	3.5229180
H	-1.1949170	0.6763420	2.7275980
N	0.0249590	4.0158840	2.1809530
H	0.2740640	4.1714410	3.1529900
C	0.9933080	4.5239790	1.2234910
C	0.4781870	5.7798010	0.4954920
H	0.2888780	6.5853250	1.2105990
H	-0.4521240	5.5371390	-0.0216550
H	1.2022890	6.1343740	-0.2439830
C	-6.2072810	-2.0977800	3.8679940

H	-7.4004790	3.2012920	2.0244640
H	-1.8644430	1.0363430	4.3358310
H	-0.2404240	1.6113660	3.9040830
H	1.1942290	3.7411800	0.4824760
H	-6.5959980	-2.9238880	4.4675350
H	-5.6570020	-2.5051220	3.0149410
H	-5.5133680	-1.5198070	4.4857120
C	2.2754370	4.8215610	2.0244330
N	3.3856670	5.0342970	1.2795270
H	3.3145540	4.9605310	0.2743250
O	2.2523050	4.8783920	3.2547320
N	8.2144470	3.8677250	1.5913370
N	16.7766360	-2.9007750	-1.7762920
O	8.5607500	5.2068570	-0.2264390
O	7.7975510	2.4668080	3.3473760
O	17.1645010	-1.4723690	-3.5262960
O	16.3336870	-4.2799250	0.0076150
C	8.8885690	4.2111120	0.4109440
C	9.9967720	3.3248040	-0.0088160
C	10.3244800	2.1673680	0.7386860
C	9.5822630	1.8511350	1.9026170
C	8.4713890	2.7187790	2.3546830
C	9.8971680	0.7155770	2.6300900
H	9.3188360	0.4866360	3.5181150
C	10.9437240	-0.1189040	2.2255590
H	11.1527420	-0.9946000	2.8270890
C	11.7047920	0.1532030	1.0867180
C	11.3967310	1.3211880	0.3185670
C	12.1345620	1.6638270	-0.8592140
C	11.7732290	2.8135510	-1.5648210
C	10.7193040	3.6329950	-1.1493450
H	10.4544390	4.5211530	-1.7119180
C	13.2438540	0.7986270	-1.2856680
C	14.0160190	1.0769790	-2.4153640
H	13.8127940	1.9560080	-3.0142090
C	15.0692480	0.2466770	-2.8132240
H	15.6575340	0.4816870	-3.6928690
C	15.3784220	-0.8917260	-2.0883290
C	14.6234480	-1.2134020	-0.9368370
C	13.5484500	-0.3703540	-0.5194850
C	12.8069110	-0.7179300	0.6533330
C	13.1599350	-1.8769160	1.3477190
C	14.2119950	-2.6980110	0.9282680
H	14.4683100	-3.5941260	1.4816980
C	14.9448230	-2.3782890	-0.2024240
C	16.0551200	-3.2664130	-0.6240030
C	16.5018220	-1.7539510	-2.5330550
C	7.1302160	4.7579020	2.0383980
H	7.4104620	5.7699730	1.7434250
C	5.7749880	4.3777310	1.4311950
H	5.4982780	3.3691450	1.7546280
H	5.8664560	4.3679820	0.3385480
C	17.8980250	-3.8021280	-2.1920460
H	17.8706720	-4.5917670	-1.4422770
C	19.2558170	-3.0982940	-2.0923540
H	19.4022930	-2.6782300	-1.0924600
H	19.3507780	-2.2997140	-2.8291290
C	17.6378280	-4.4382990	-3.5619000
H	17.6725050	-3.6995430	-4.3633990
H	16.6634720	-4.9362460	-3.5799490
H	12.3101830	3.0964860	-2.4614640
H	12.6174590	-2.1678370	2.2385620
C	4.6851440	5.3693160	1.8519640
H	20.0501740	-3.8308390	-2.2674250
H	18.4044720	-5.1961400	-3.7523130
H	7.0923160	4.6926650	3.1261080

H	4.9652570	6.3868970	1.5501320
H	4.5522080	5.3691890	2.9357410
H	-6.9753390	-0.6408900	-1.8621770

Folded Cor-(Ala)$_4$-PDI$_{opt}$ with hydrogen bond to PDI in chloroform

Energy total = -5475.33455241 a.u.

Symbol	X	Y	Z
O	-3.4783740	2.5676580	4.0698280
C	-2.7233040	1.9138720	5.0774560
H	-3.3748740	1.4345230	5.8186530
H	-2.0646690	2.6146870	5.6053340
C	-1.8606650	0.8172140	4.4523070
O	-1.1210100	0.1491910	5.1760520
N	-1.9892800	0.6453530	3.1209280
H	-2.6267240	1.2299720	2.5935730
C	-1.3338590	-0.4394320	2.4129780
H	-0.3004450	-0.5198130	2.7648400
C	-1.3378070	-0.1076270	0.9138920
O	-2.0805990	0.7733390	0.4553790
N	-0.5248510	-0.8792600	0.1621780
H	0.0787950	-1.5572020	0.6251670
C	-0.5537570	-0.8860970	-1.2942580
H	-1.3143870	-0.1676680	-1.5970230
C	0.8021480	-0.4824530	-1.8940760
H	1.5878780	-1.1655160	-1.5594620
H	0.7632280	-0.5105420	-2.9869320
C	-2.0404840	-1.7878720	2.6664600
H	1.0568770	0.5342340	-1.5839690
H	-2.0437920	-1.9864330	3.7400050
H	-3.0739810	-1.7513410	2.3093370
H	-1.5178650	-2.6045220	2.1641760
C	-0.9489270	-2.2919140	-1.7753840
O	-0.4432930	-3.3008090	-1.2746980
N	-1.8588980	-2.3466560	-2.7776500
H	-2.2307090	-1.4796030	-3.1467630
C	-2.1634240	-3.5821860	-3.5151080
C	-2.6632120	-4.7198490	-2.5895450
O	-2.3565790	-5.8888550	-2.7997930
C	-0.9939700	-4.0476000	-4.3845140
H	-0.1264100	-4.2799700	-3.7640710
H	-0.7263990	-3.2653210	-5.0997050
H	-1.2746060	-4.9493840	-4.9303250
N	-3.4957240	-4.3266180	-1.5885930
H	-3.7224900	-3.3446610	-1.5250460
C	-4.1657380	-5.2364310	-0.6556180
C	-5.0735600	-6.2616220	-1.3454420
C	-3.2235480	-5.9041860	0.3741600
O	-3.6622530	-6.7845170	1.1184160
H	-3.0122260	-3.3265260	-4.1602880
H	-4.8049760	-4.5902140	-0.0448430
H	-5.5118170	-6.9123720	-0.5872600
H	-4.5052470	-6.8692680	-2.0506760
H	-5.8766220	-5.7438160	-1.8753730
N	-1.9698950	-5.4131090	0.4690200
H	-1.6608250	-4.6914050	-0.1722050
N	2.4795170	-4.4446830	2.1443520
N	12.2694880	0.7291530	-0.6520780
O	1.3665100	-2.4714860	1.8905530
O	3.5875870	-6.4384570	2.3231540
O	11.1237990	2.7027550	-0.8559940
O	13.3509460	-1.2863720	-0.4372810
C	2.4394610	-3.0828720	1.8558330
C	3.7131750	-2.4204700	1.5131830
C	4.9190820	-3.1613070	1.4572050

C	4.9027890	-4.5482090	1.7403420
C	3.6414110	-5.2367820	2.0899280
C	6.0817220	-5.2738990	1.6844040
H	6.0550060	-6.3351620	1.9038490
C	7.2856440	-4.6476870	1.3488680
H	8.1804730	-5.2560150	1.3187890
C	7.3493090	-3.2832130	1.0575350
C	6.1445010	-2.5125400	1.1119510
C	6.1348270	-1.1093520	0.8295000
C	4.9231110	-0.4185770	0.9045440
C	3.7285060	-1.0618990	1.2399580
H	2.8002840	-0.5043690	1.2890190
C	7.3947040	-0.4434370	0.4688380
C	7.4601890	0.9204880	0.1763330
H	6.5669680	1.5311680	0.2104750
C	8.6637030	1.5442620	-0.1691210
H	8.6909450	2.6045180	-0.3926700
C	9.8397800	0.8158220	-0.2316390
C	9.8208310	-0.5684760	0.0568140
C	8.5974460	-1.2153400	0.4109870
C	8.6088990	-2.6169720	0.6959760
C	9.8212270	-3.3055660	0.6173060
C	11.0138990	-2.6624310	0.2700560
H	11.9433220	-3.2172830	0.2153280
C	11.0254510	-1.3060790	-0.0099130
C	12.3031330	-0.6503870	-0.3764960
C	11.1022700	1.5019840	-0.6022580
C	1.1990830	-5.1043080	2.4714950
H	0.6546420	-4.4277520	3.1326310
C	0.3744390	-5.3869000	1.2103850
H	0.8717730	-6.1481420	0.6005210
H	0.3429360	-4.4704010	0.6175810
C	13.5664940	1.3817450	-1.0196590
H	14.2783510	0.5588380	-0.9722860
C	13.9875780	2.4316720	0.0142180
H	13.9982010	2.0022620	1.0207390
H	13.3231790	3.2964490	0.0063430
C	13.5488500	1.9094850	-2.4584180
H	12.8664300	2.7526740	-2.5720870
H	13.2560730	1.1199890	-3.1574100
H	4.8850920	0.6438560	0.7009760
H	9.8625020	-4.3671720	0.8252320
C	-1.0629690	-5.8150970	1.5398000
H	15.0028000	2.7695190	-0.2168540
H	14.5573970	2.2388200	-2.7278420
H	1.4429880	-6.0166240	3.0136450
H	-1.3887380	-5.3507520	2.4823520
H	-1.1460940	-6.8958910	1.6838740
C	-3.6611720	0.8269890	-3.1503550
C	-4.2963150	-0.1032600	-4.0183310
H	-3.9615760	-0.3667350	-5.0124150
C	-5.4373910	-0.5771070	-3.3689310
H	-6.1585750	-1.2756640	-3.7687810
C	-5.5184650	0.0686770	-2.1011810
C	-6.4861450	0.1171120	-1.0627500
C	-6.3937810	1.0325080	0.0112600
C	-7.2694590	1.0677790	1.1713260
H	-8.1188590	0.4221770	1.3458150
C	-6.7882630	2.0345920	1.9974270
H	-7.1810540	2.3345550	2.9581700
C	-5.6169190	2.6074590	1.3443360
C	-4.8009730	3.6178560	1.9244000
C	-3.6431940	4.1749910	1.3588670
C	-2.7105430	5.0912330	1.9562240
H	-2.8154390	5.5128440	2.9445200
C	-1.6782310	5.2973700	1.0779520

H	-0.8004920	5.9047890	1.2432140
C	-1.9235270	4.5262910	-0.1086100
C	-1.1213660	4.3967780	-1.2564550
C	-1.4067180	3.4488020	-2.2775600
C	-1.1231130	3.4229460	-3.6640210
H	-0.5339980	4.1585670	-4.1930810
C	-1.8394650	2.3683480	-4.2388810
H	-1.9115150	2.1412400	-5.2933750
C	-2.5622350	1.7282530	-3.2125540
N	-4.4138930	0.8633020	-2.0098450
H	-4.3614030	1.5036880	-1.2064810
N	-5.4093860	1.9935570	0.1446800
N	-3.1327960	3.8854560	0.1140930
N	-2.2501950	2.3838340	-2.0327030
H	-2.2580570	1.9029800	-1.1275770
C	-5.1250150	4.0643190	3.3201880
C	-4.4187170	3.5030250	4.4072630
C	-4.6882670	3.9030720	5.7186670
H	-4.1414550	3.4776350	6.5518600
C	-5.6768320	4.8631630	5.9551330
H	-5.8830010	5.1687830	6.9765490
C	-6.3889440	5.4239410	4.8976640
H	-7.1548310	6.1697900	5.0841680
C	-6.1050790	5.0223080	3.5887440
H	-6.6491350	5.4563800	2.7550480
C	-7.6094910	-0.8520000	-1.1283200
C	-7.3734790	-2.2329760	-1.1350490
C	-8.3980130	-3.1684740	-1.2217630
C	-9.7179470	-2.7332680	-1.3012380
C	-9.9940230	-1.3689050	-1.2944220
C	-8.9490660	-0.4521010	-1.2165550
F	-6.1126150	-2.6998000	-1.0366180
F	-8.1251670	-4.4803320	-1.2192470
F	-10.7131940	-3.6202070	-1.3820330
F	-11.2609680	-0.9457060	-1.3819230
F	-9.2627520	0.8511020	-1.2401200
C	0.0498630	5.2850170	-1.4405960
C	1.3303960	4.7563540	-1.6648980
C	2.4451710	5.5633270	-1.8649430
C	2.3064840	6.9483120	-1.8405100
C	1.0525450	7.5102930	-1.6192080
C	-0.0512740	6.6838640	-1.4305660
F	1.5208390	3.4262330	-1.6712090
F	3.6514040	5.0162580	-2.0648160
F	3.3715100	7.7329030	-2.0267560
F	0.9110370	8.8415240	-1.6080020
F	-1.2420340	7.2737750	-1.2498320
H	-3.6547220	3.3428090	-0.5557100

Folded Cor-$(Ala)_4$-PDI_{opt} with hydrogen bond to PDI in toluene

Energy total = -5475.32309308 a.u.

Symbol	X	Y	Z
O	-3.1954090	2.6730580	4.0805840
C	-2.4509120	1.9469620	5.0454110
H	-3.1068350	1.4990430	5.8023300
H	-1.7246110	2.5880540	5.5604000
C	-1.6930730	0.8048630	4.3665820
O	-0.9690270	0.0782010	5.0459080
N	-1.8975610	0.6625810	3.0401190
H	-2.5130100	1.3001230	2.5492890
C	-1.3530620	-0.4558640	2.2927960
H	-0.3190260	-0.6245120	2.6099280
C	-1.3765840	-0.0978930	0.8004210

O	-2.0438860	0.8575010	0.3774760
N	-0.6698170	-0.9334410	0.0096470
H	-0.0996800	-1.6598770	0.4388990
C	-0.7487900	-0.9083360	-1.4431770
H	-1.5393110	-0.2045420	-1.7032190
C	0.5734940	-0.4539090	-2.0843900
H	1.3881390	-1.1225440	-1.7922770
H	0.4970900	-0.4585210	-3.1758330
C	-2.1545530	-1.7500930	2.5489840
H	0.8126980	0.5623560	-1.7604560
H	-2.1452820	-1.9618930	3.6200560
H	-3.1910660	-1.6311510	2.2190790
H	-1.7095300	-2.5986900	2.0246140
C	-1.1167910	-2.3150010	-1.9410320
O	-0.5844820	-3.3184030	-1.4596420
N	-2.0253790	-2.3730470	-2.9458900
H	-2.4310220	-1.5078040	-3.2821630
C	-2.2715450	-3.5918340	-3.7334410
C	-2.7452460	-4.7860550	-2.8645410
O	-2.3837960	-5.9293130	-3.1165220
C	-1.0688200	-3.9805520	-4.5952580
H	-0.2086520	-4.2115890	-3.9642950
H	-0.8116710	-3.1599780	-5.2708850
H	-1.3058250	-4.8680800	-5.1834400
N	-3.6208560	-4.4670970	-1.8730460
H	-3.8709470	-3.4950430	-1.7612850
C	-4.2679320	-5.4348260	-0.9811780
C	-5.0613390	-6.5191550	-1.7204630
C	-3.3358030	-6.0495800	0.0897140
O	-3.7706390	-6.9273370	0.8367110
H	-3.1167760	-3.3428840	-4.3863320
H	-4.9835550	-4.8454780	-0.4000970
H	-5.5023470	-7.1922050	-0.9837200
H	-4.4112290	-7.0903160	-2.3835220
H	-5.8620350	-6.0593270	-2.3061830
N	-2.0975100	-5.5223380	0.2075100
H	-1.7892780	-4.8032680	-0.4361890
N	2.3262470	-4.5322210	1.9739350
N	12.2331670	0.6348160	-0.3990230
O	1.2327070	-2.5490840	1.7097420
O	3.4189730	-6.5348760	2.1537320
O	11.1072980	2.6223750	-0.5813080
O	13.2934810	-1.3936820	-0.1985260
C	2.3011760	-3.1675880	1.6997140
C	3.5893940	-2.5073850	1.4052650
C	4.7928150	-3.2537150	1.3753000
C	4.7596210	-4.6450510	1.6336340
C	3.4845670	-5.3316150	1.9384280
C	5.9347950	-5.3775120	1.6001020
H	5.8928510	-6.4422250	1.8000940
C	7.1520840	-4.7528400	1.3128660
H	8.0441890	-5.3660040	1.2986510
C	7.2337440	-3.3835390	1.0504180
C	6.0323500	-2.6061810	1.0818310
C	6.0397100	-1.1976120	0.8271840
C	4.8287790	-0.5028510	0.8703800
C	3.6200980	-1.1453140	1.1535270
H	2.6921870	-0.5856150	1.1802230
C	7.3155680	-0.5312230	0.5286020
C	7.4008490	0.8396950	0.2768320
H	6.5108780	1.4559390	0.2994320
C	8.6194820	1.4639070	-0.0102410
H	8.6636640	2.5297330	-0.2030090
C	9.7916170	0.7282860	-0.0538110
C	9.7535900	-0.6630870	0.1961940
C	8.5147900	-1.3100190	0.4921060

C	8.5081550	-2.7182860	0.7428090
C	9.7181750	-3.4129210	0.6852150
C	10.9258800	-2.7701780	0.3931560
H	11.8541400	-3.3284580	0.3533070
C	10.9550940	-1.4072980	0.1498010
C	12.2495410	-0.7517230	-0.1570630
C	11.0705990	1.4157570	-0.3637740
C	1.0357990	-5.1870220	2.2704690
H	0.4832310	-4.5114130	2.9261190
C	0.2309220	-5.4580250	0.9946680
H	0.7361990	-6.2147490	0.3856730
H	0.2058600	-4.5366840	0.4087710
C	13.5452270	1.2866200	-0.7098550
H	14.2489860	0.4563730	-0.6663060
C	13.9428460	2.3031640	0.3659310
H	13.9249990	1.8437730	1.3590650
H	13.2821260	3.1708380	0.3657470
C	13.5716440	1.8575960	-2.1319180
H	12.8987900	2.7093500	-2.2384670
H	13.2931200	1.0919010	-2.8625580
H	4.8032510	0.5629290	0.6821630
H	9.7451590	-4.4798280	0.8675600
C	-1.2090210	-5.8901490	1.3040810
H	14.9653720	2.6430130	0.1728150
H	14.5897350	2.1864600	-2.3635450
H	1.2652480	-6.1046120	2.8103830
H	-1.5562290	-5.4071200	2.2299060
H	-1.2875970	-6.9679210	1.4714940
C	-3.7471500	0.9520020	-3.1181590
C	-4.4160140	0.0028780	-3.9378400
H	-4.1489000	-0.2510900	-4.9547930
C	-5.4981790	-0.4975320	-3.2091210
H	-6.2288570	-1.2141890	-3.5563990
C	-5.5088570	0.1531120	-1.9425590
C	-6.4022230	0.1791740	-0.8375610
C	-6.2692240	1.1080140	0.2179660
C	-7.0764540	1.1371720	1.4273990
H	-7.9016980	0.4773250	1.6552920
C	-6.5707810	2.1242280	2.2126710
H	-6.9142000	2.4294960	3.1904540
C	-5.4502830	2.7127030	1.4864950
C	-4.6171830	3.7383620	2.0137860
C	-3.4982510	4.3025870	1.3827780
C	-2.5426140	5.2304400	1.9242880
H	-2.5973230	5.6545750	2.9155710
C	-1.5636110	5.4429250	0.9892950
H	-0.6843120	6.0597780	1.1026890
C	-1.8674320	4.6655110	-0.1799550
C	-1.1331580	4.5436900	-1.3720340
C	-1.4705880	3.5944980	-2.3772800
C	-1.2760430	3.5799250	-3.7784120
H	-0.7302830	4.3255460	-4.3390130
C	-2.0172660	2.5208660	-4.3135700
H	-2.1562400	2.3008200	-5.3629190
C	-2.6652490	1.8674490	-3.2480480
N	-4.4249100	0.9785570	-1.9319270
H	-4.3293260	1.6166750	-1.1305740
N	-5.3011860	2.0927960	0.2826790
N	-3.0547520	4.0120240	0.1131690
N	-2.2841140	2.5181170	-2.0862250
H	-2.2382690	2.0318370	-1.1853140
C	-4.8656990	4.1852700	3.4249250
C	-4.1117860	3.6101920	4.4719170
C	-4.3117610	4.0037220	5.7975280
H	-3.7269350	3.5679870	6.5991700
C	-5.2770110	4.9723300	6.0885770

H	-5.4293400	5.2733480	7.1207860
C	-6.0335390	5.5483930	5.0711310
H	-6.7809660	6.3010970	5.3001160
C	-5.8196420	5.1525960	3.7471850
H	-6.4002830	5.5972320	2.9442830
C	-7.4709800	-0.8515450	-0.8069270
C	-7.1455770	-2.2136820	-0.7918190
C	-8.1066330	-3.2175360	-0.7949000
C	-9.4553850	-2.8706310	-0.8044070
C	-9.8202040	-1.5266530	-0.8125670
C	-8.8362590	-0.5405890	-0.8200290
F	-5.8506560	-2.5903460	-0.7482490
F	-7.7431150	-4.5070600	-0.7758470
F	-10.3931470	-3.8205260	-0.8042470
F	-11.1151190	-1.1905480	-0.8314120
F	-9.2347650	0.7381920	-0.8503590
C	0.0156190	5.4440780	-1.6253060
C	1.2849420	4.9279440	-1.9296040
C	2.3778470	5.7461100	-2.1957270
C	2.2278360	7.1299320	-2.1592100
C	0.9844040	7.6795580	-1.8596050
C	-0.0982970	6.8421790	-1.6057400
F	1.4865300	3.6002290	-1.9508330
F	3.5743250	5.2110250	-2.4706800
F	3.2715870	7.9250100	-2.4082900
F	0.8317190	9.0089170	-1.8358750
F	-1.2807020	7.4201080	-1.3505560
H	-3.6079460	3.4605560	-0.5233520

Folded Cor-(Ala)$_4$-PDI$_{opt}$ without hydrogen bond to PDI in chloroform

Energy total = -5475.33298688 a.u.

Symbol	X	Y	Z
C	-4.4809710	1.6218700	-2.5455380
C	-5.5603700	0.8446280	-3.0468230
H	-5.7853550	0.6795870	-4.0919300
C	-6.2891180	0.3758650	-1.9515000
H	-7.1897690	-0.2204100	-1.9884560
C	-5.6703670	0.8748740	-0.7691750
C	-5.9973270	0.8637340	0.6127910
C	-5.2964710	1.6435380	1.5611380
C	-5.4973170	1.6084260	3.0008140
H	-6.2269280	1.0072050	3.5250990
C	-4.5757000	2.4462330	3.5465510
H	-4.4248110	2.6667830	4.5933820
C	-3.8046290	3.0069130	2.4425610
C	-2.6984230	3.8853060	2.6125100
C	-1.8960720	4.4132610	1.5884840
C	-0.7000140	5.2012340	1.7079070
H	-0.2708970	5.5236850	2.6446510
C	-0.2039920	5.4341260	0.4512940
H	0.7024760	5.9661150	0.2023660
C	-1.0704100	4.8086860	-0.5078780
C	-0.9457880	4.7609330	-1.9077350
C	-1.7875330	3.9498800	-2.7176430
C	-2.2216070	4.0751940	-4.0593110
H	-1.8856120	4.8323190	-4.7534630
C	-3.2444240	3.1477850	-4.2788890
H	-3.8499310	3.0580490	-5.1699010
C	-3.4443350	2.4352490	-3.0804120
N	-4.5789110	1.5798830	-1.1825810
H	-4.0677240	2.1164380	-0.4698620
N	-4.2688100	2.5166190	1.2577690
N	-2.0795110	4.2186950	0.2384930
N	-2.5189530	2.9151970	-2.1681190

H	-2.1550130	2.3322820	-1.4106080
C	-2.2655430	4.2045390	4.0136240
C	-1.1928760	3.4888370	4.5885930
C	-0.7635760	3.7629480	5.8895720
H	0.0710620	3.2232140	6.3220550
C	-1.4148140	4.7505770	6.6344790
H	-1.0781410	4.9587400	7.6456250
C	-2.4787390	5.4645650	6.0877910
H	-2.9813940	6.2321220	6.6672930
C	-2.8925470	5.1892510	4.7811220
H	-3.7181370	5.7420540	4.3427710
C	-7.1012640	-0.0322890	1.0418450
C	-7.0256870	-1.4153810	0.8347320
C	-8.0507760	-2.2844630	1.1883880
C	-9.2037780	-1.7778130	1.7821430
C	-9.3144380	-0.4089660	2.0106130
C	-8.2770910	0.4415090	1.6367420
F	-5.9120160	-1.9514670	0.2917420
F	-7.9307220	-3.6025570	0.9735760
F	-10.1961310	-2.6001420	2.1310530
F	-10.4246680	0.0844090	2.5717090
F	-8.4393730	1.7540650	1.8538340
C	0.0614070	5.6126980	-2.5830790
C	1.0149980	5.0579070	-3.4503140
C	1.9590390	5.8344120	-4.1138840
C	1.9755420	7.2129240	-3.9209030
C	1.0452180	7.8000360	-3.0682850
C	0.1036260	7.0053680	-2.4213250
F	1.0525000	3.7312620	-3.6489380
F	2.8592720	5.2630190	-4.9240110
F	2.8799650	7.9680520	-4.5504430
F	1.0483760	9.1271670	-2.8904290
F	-0.7902890	7.6221520	-1.6342600
O	-0.6178690	2.5457460	3.7776550
C	0.2603850	1.5697390	4.3161060
H	-0.0920560	1.2086410	5.2897850
H	1.2740430	1.9674170	4.4449290
C	0.3247160	0.3565350	3.3864720
O	1.0876780	-0.5702070	3.6674980
N	-0.5056070	0.3847970	2.3255190
H	-1.0777400	1.2063860	2.1700190
C	-0.7088460	-0.7506390	1.4455760
H	0.2370840	-1.2945490	1.3630170
C	-1.1266060	-0.2255990	0.0628590
O	-1.4891660	0.9456280	-0.1031770
N	-1.1162280	-1.1493390	-0.9218970
H	-0.8057090	-2.0953700	-0.7370090
C	-1.6744420	-0.9186430	-2.2469620
H	-2.3996540	-0.1082240	-2.1575970
C	-0.5985300	-0.5332990	-3.2772910
H	0.1417590	-1.3322170	-3.3723100
H	-1.0492540	-0.3555250	-4.2580440
C	-1.7791140	-1.7085890	2.0111800
H	-0.0946590	0.3816460	-2.9568930
H	-1.4516980	-2.0715570	2.9873960
H	-2.7348790	-1.1882310	2.1241470
H	-1.9272210	-2.5745800	1.3613140
C	-2.3766240	-2.2135060	-2.6764970
O	-1.8714710	-3.3125690	-2.4230540
N	-3.5407380	-2.0611920	-3.3482450
H	-3.8902310	-1.1212140	-3.4885740
C	-4.2100340	-3.1515090	-4.0735370
C	-4.5690140	-4.3494110	-3.1613620
O	-4.5598790	-5.4961210	-3.5988630
C	-3.4154560	-3.6058700	-5.2998860
H	-2.4421610	-3.9994820	-4.9998560

H	-3.2676820	-2.7639610	-5.9812550
H	-3.9581700	-4.3963230	-5.8195710
N	-4.9354280	-4.0319760	-1.8923810
H	-4.9316180	-3.0587380	-1.6231360
C	-5.3708330	-5.0124920	-0.8951910
C	-6.6419150	-5.7670650	-1.3017540
C	-4.2582050	-5.9853430	-0.4379870
O	-4.5543910	-6.9771460	0.2321420
H	-5.1673380	-2.7309750	-4.4032280
H	-5.6047110	-4.4242620	-0.0025640
H	-6.8934310	-6.4860710	-0.5209970
H	-6.4883610	-6.3021960	-2.2396940
H	-7.4703520	-5.0634010	-1.4177750
N	-2.9810250	-5.6399520	-0.7137420
H	-2.7809100	-4.8687600	-1.3415230
N	1.8160720	-5.5511450	0.4773860
N	11.6518750	0.2554330	0.5573740
O	0.9160390	-4.0404290	1.9302600
O	2.6998860	-7.0150320	-1.0442600
O	10.7233040	1.7370520	2.0377930
O	12.5169450	-1.2648420	-0.9321060
C	1.8872200	-4.3960530	1.2665270
C	3.1619430	-3.6465800	1.2589890
C	4.2527780	-4.0868840	0.4700850
C	4.1167930	-5.2474440	-0.3300650
C	2.8506830	-6.0154870	-0.3492050
C	5.1821270	-5.6748070	-1.1056150
H	5.0638710	-6.5642400	-1.7139760
C	6.3907950	-4.9718290	-1.1014680
H	7.1952060	-5.3457310	-1.7220460
C	6.5713210	-3.8232930	-0.3275700
C	5.4833000	-3.3604110	0.4782520
C	5.5938160	-2.1883500	1.2926460
C	4.4882110	-1.7901490	2.0463400
C	3.2853120	-2.5050440	2.0352310
H	2.4439370	-2.1612700	2.6285660
C	6.8621000	-1.4450820	1.3070560
C	7.0452220	-0.2978130	2.0820280
H	6.2409430	0.0761430	2.7027510
C	8.2563380	0.4016890	2.0898510
H	8.3760380	1.2898850	2.6995770
C	9.3231840	-0.0301650	1.3192150
C	9.1835450	-1.1881160	0.5194520
C	7.9505860	-1.9097950	0.5034060
C	7.8388370	-3.0781960	-0.3145190
C	8.9437550	-3.4717730	-1.0725610
C	10.1464110	-2.7582310	-1.0494820
H	10.9911990	-3.0838430	-1.6454000
C	10.2771420	-1.6248740	-0.2637350
C	11.5634890	-0.8898780	-0.2558400
C	10.5963750	0.7296330	1.3474480
C	0.5539920	-6.3152460	0.5154910
H	0.2596330	-6.3997460	1.5638010
C	-0.5621060	-5.6411790	-0.2876910
H	-0.2454780	-5.5071370	-1.3276140
H	-0.7390780	-4.6489330	0.1352030
C	12.9581360	0.9876850	0.5622820
H	13.5693980	0.4054560	-0.1258070
C	13.6265890	0.9461240	1.9408590
H	13.7186030	-0.0847330	2.2964720
H	13.0691110	1.5256380	2.6776620
C	12.8203780	2.4031570	-0.0091920
H	12.2351820	3.0486110	0.6467600
H	12.3479940	2.3790040	-0.9961020
H	4.5368550	-0.9040420	2.6665230
H	8.8908010	-4.3514550	-1.7013240

C	-1.8641570	-6.4430690	-0.2295150
H	14.6350990	1.3639130	1.8592530
H	13.8185190	2.8370520	-0.1260900
H	0.7796210	-7.3067540	0.1248920
H	-2.0908160	-6.7416490	0.7996240
H	-1.7724380	-7.3697930	-0.8121060
H	-2.9196620	3.7941090	-0.1213920

Folded Cor-(Ala)$_4$-PDI$_{opt}$ without hydrogen bond to PDI in toluene

Energy total = -5475.32158714 a.u.

Symbol	X	Y	Z
C	-4.5220600	1.5954300	-2.5137320
C	-5.6012250	0.8100380	-3.0015450
H	-5.8428590	0.6496140	-4.0437730
C	-6.3107930	0.3320380	-1.8965700
H	-7.2082110	-0.2697070	-1.9222280
C	-5.6793780	0.8326370	-0.7226790
C	-5.9866880	0.8160320	0.6644600
C	-5.2815420	1.6023040	1.6030960
C	-5.4632300	1.5646120	3.0455740
H	-6.1790760	0.9551400	3.5790820
C	-4.5452720	2.4129620	3.5794060
H	-4.3833100	2.6354020	4.6240860
C	-3.7956260	2.9837270	2.4651820
C	-2.7006240	3.8789400	2.6218300
C	-1.9191430	4.4181960	1.5878450
C	-0.7346720	5.2260070	1.6922920
H	-0.3013300	5.5579900	2.6236610
C	-0.2570800	5.4639770	0.4301870
H	0.6371910	6.0106840	0.1695780
C	-1.1243900	4.8226910	-0.5181610
C	-1.0143620	4.7744140	-1.9185410
C	-1.8567300	3.9536250	-2.7186820
C	-2.3097840	4.0760390	-4.0536520
H	-1.9913770	4.8378140	-4.7509640
C	-3.3257930	3.1379710	-4.2607410
H	-3.9428230	3.0445230	-5.1434460
C	-3.5015290	2.4215330	-3.0613030
N	-4.5999820	1.5477750	-1.1496940
H	-4.0842580	2.0871660	-0.4418820
N	-4.2675810	2.4869460	1.2868770
N	-2.1155740	4.2191860	0.2409390
N	-2.5690170	2.9102040	-2.1609840
H	-2.1889860	2.3317130	-1.4075270
C	-2.2560260	4.2062220	4.0173250
C	-1.1481320	3.5273130	4.5698540
C	-0.7068960	3.8097620	5.8649020
H	0.1549470	3.2988810	6.2789260
C	-1.3815090	4.7674800	6.6274830
H	-1.0355680	4.9822470	7.6341250
C	-2.4805350	5.4440820	6.1036140
H	-3.0014660	6.1887460	6.6966740
C	-2.9058990	5.1619040	4.8022710
H	-3.7586490	5.6864300	4.3815470
C	-7.0773990	-0.0897510	1.1063180
C	-6.9963830	-1.4714210	0.8905740
C	-8.0109420	-2.3491480	1.2540670
C	-9.1584500	-1.8527790	1.8676000
C	-9.2740230	-0.4856500	2.1055480
C	-8.2475770	0.3737420	1.7209770
F	-5.8875020	-1.9977410	0.3282880
F	-7.8860950	-3.6646000	1.0296620
F	-10.1403110	-2.6827040	2.2259490
F	-10.3785180	-0.0025550	2.6853350

F	-8.4149270	1.6834070	1.9471600
C	-0.0235740	5.6350200	-2.6068690
C	0.9264280	5.0867170	-3.4824420
C	1.8552110	5.8707180	-4.1591140
C	1.8592670	7.2503180	-3.9709830
C	0.9319100	7.8310080	-3.1102670
C	0.0054520	7.0287830	-2.4501750
F	0.9752130	3.7601520	-3.6765590
F	2.7521960	5.3060780	-4.9767340
F	2.7487320	8.0122630	-4.6125680
F	0.9232610	9.1582330	-2.9371100
F	-0.8859160	7.6383620	-1.6555410
O	-0.5524270	2.6113120	3.7432660
C	0.3581750	1.6539360	4.2598780
H	0.0373900	1.2859750	5.2420870
H	1.3666210	2.0716780	4.3636400
C	0.4244520	0.4407640	3.3294780
O	1.2276070	-0.4591010	3.5812740
N	-0.4529770	0.4384770	2.3063670
H	-1.0470450	1.2468850	2.1650630
C	-0.6576660	-0.7068880	1.4400670
H	0.2952500	-1.2345910	1.3378390
C	-1.1179400	-0.2007150	0.0644460
O	-1.4905080	0.9664890	-0.1063390
N	-1.1299960	-1.1349550	-0.9115070
H	-0.8105030	-2.0781530	-0.7273460
C	-1.7097460	-0.9069120	-2.2274700
H	-2.4441100	-0.1064900	-2.1230710
C	-0.6534320	-0.5003970	-3.2701750
H	0.0946760	-1.2898290	-3.3821420
H	-1.1194880	-0.3203740	-4.2434380
C	-1.6917480	-1.6818760	2.0417000
H	-0.1560360	0.4182790	-2.9503490
H	-1.3365420	-2.0149890	3.0188070
H	-2.6603510	-1.1869010	2.1604550
H	-1.8211060	-2.5669510	1.4143270
C	-2.4009340	-2.2071490	-2.6577910
O	-1.8778760	-3.3009170	-2.4244590
N	-3.5770320	-2.0604310	-3.3126080
H	-3.9438460	-1.1232510	-3.4264930
C	-4.2416010	-3.1470060	-4.0485250
C	-4.5910540	-4.3621080	-3.1538890
O	-4.5906910	-5.4976040	-3.6161830
C	-3.4487780	-3.5818340	-5.2831810
H	-2.4707270	-3.9691360	-4.9906110
H	-3.3120200	-2.7332010	-5.9588420
H	-3.9859400	-4.3747170	-5.8046570
N	-4.9393090	-4.0674580	-1.8737460
H	-4.9226950	-3.1001570	-1.5851460
C	-5.3537710	-5.0661350	-0.8846230
C	-6.6213120	-5.8291520	-1.2861480
C	-4.2282290	-6.0349910	-0.4495100
O	-4.5077060	-7.0211780	0.2329440
H	-5.2029520	-2.7281790	-4.3694270
H	-5.5835330	-4.4917690	0.0181260
H	-6.8499660	-6.5640610	-0.5131920
H	-6.4742580	-6.3464940	-2.2349380
H	-7.4607150	-5.1345930	-1.3781000
N	-2.9575660	-5.6893010	-0.7579420
H	-2.7714300	-4.9200790	-1.3912160
N	1.8384660	-5.5384910	0.4120370
N	11.6732710	0.2708250	0.5838650
O	0.8864610	-3.9569940	1.7521700
O	2.7685440	-7.0569220	-1.0270220
O	10.7085710	1.7872350	2.0056270
O	12.5730860	-1.2868560	-0.8457530

C	1.8831180	-4.3493150	1.1499940
C	3.1641560	-3.6101680	1.1697060
C	4.2753290	-4.0728340	0.4229850
C	4.1591600	-5.2555720	-0.3470100
C	2.8963290	-6.0307360	-0.3691800
C	5.2432950	-5.7041720	-1.0831800
H	5.1386970	-6.6116470	-1.6671240
C	6.4512450	-4.9999030	-1.0687270
H	7.2710840	-5.3896820	-1.6588760
C	6.6140410	-3.8316990	-0.3206980
C	5.5068600	-3.3483190	0.4459840
C	5.5994280	-2.1588040	1.2372690
C	4.4774820	-1.7455670	1.9576390
C	3.2722830	-2.4563350	1.9293450
H	2.4216160	-2.0998280	2.5018030
C	6.8677070	-1.4159670	1.2646420
C	7.0335580	-0.2506760	2.0161670
H	6.2143370	0.1369340	2.6085640
C	8.2441110	0.4496820	2.0354090
H	8.3519150	1.3526050	2.6256110
C	9.3279710	0.0002360	1.2997810
C	9.2068080	-1.1766920	0.5251950
C	7.9744670	-1.8992460	0.4976780
C	7.8815610	-3.0866300	-0.2949830
C	9.0042290	-3.4969480	-1.0172200
C	10.2063880	-2.7827720	-0.9828970
H	11.0661370	-3.1202370	-1.5503530
C	10.3184530	-1.6312220	-0.2215660
C	11.6050920	-0.8953340	-0.2020690
C	10.5997730	0.7632770	1.3382560
C	0.5817700	-6.3115670	0.4573740
H	0.2678290	-6.3506910	1.5029210
C	-0.5287550	-5.6882830	-0.3928320
H	-0.2059510	-5.6139270	-1.4368800
H	-0.7108830	-4.6736870	-0.0304300
C	12.9776510	1.0060380	0.5982970
H	13.6051790	0.4070890	-0.0604320
C	13.6140880	1.0039990	1.9925600
H	13.7030790	-0.0167850	2.3769030
H	13.0364940	1.5995650	2.7004950
C	12.8482530	2.4057890	-0.0126780
H	12.2446580	3.0648040	0.6123950
H	12.4003640	2.3541850	-1.0099340
H	4.5120650	-0.8498260	2.5649670
H	8.9652500	-4.3911880	-1.6264550
C	-1.8306650	-6.4879930	-0.2917850
H	14.6223550	1.4248180	1.9236030
H	13.8470720	2.8415090	-0.1168700
H	0.8248780	-7.3174240	0.1166720
H	-2.0335770	-6.7718240	0.7467320
H	-1.7563890	-7.4238260	-0.8619410
H	-2.9513170	3.7765570	-0.1069700

Turn1,4-Cor-(Ala)$_4$-PDI$_{opt}$ in chloroform

Energy total = -5475.32413890 a.u.

Symbol	X	Y	Z
C	9.0564150	2.8879030	-0.9033970
C	9.7374940	4.0874770	-1.2328860
H	10.7957730	4.1733330	-1.4350550
C	8.8186460	5.1343180	-1.1647820
H	9.0309660	6.1848110	-1.3034250
C	7.5532530	4.5957520	-0.7902190
C	6.3089430	5.1739230	-0.4208970

C	5.3303470	4.4524410	0.2931250
C	3.9538980	4.7591720	0.5003480
H	3.4521590	5.6258840	0.0947500
C	3.3734350	3.7429470	1.2263710
H	2.3338730	3.6648160	1.5081780
C	4.3607400	2.7493200	1.5071210
C	4.1868210	1.5256970	2.1748210
C	5.1115700	0.4550400	2.2519290
C	4.9517640	-0.7766790	2.9696790
H	4.0950040	-1.0202270	3.5800940
C	6.0639930	-1.5611130	2.7539620
H	6.2448090	-2.5481490	3.1541340
C	6.9529010	-0.8420500	1.8976760
C	8.2229460	-1.1840940	1.3759560
C	8.9432620	-0.3197870	0.5180620
C	10.3215330	-0.4031860	0.0666300
H	11.0047330	-1.2228650	0.2438890
C	10.5969050	0.7754530	-0.5819200
H	11.5319860	1.0733240	-1.0373000
C	9.3832010	1.5534780	-0.5307810
N	7.7508130	3.2448670	-0.6988210
H	7.0300330	2.5537970	-0.5726600
N	5.5370110	3.2033100	0.9035020
H	6.4403520	2.9787970	1.3008690
N	6.3358840	0.3641940	1.6284070
N	8.4062040	0.8655370	0.1069200
C	2.8627710	1.3184950	2.8512710
C	1.8244270	0.6163920	2.2018690
C	0.5912020	0.4263950	2.8335280
H	-0.2048570	-0.1174220	2.3394870
C	0.3853950	0.9384230	4.1171290
H	-0.5748730	0.7836390	4.5998220
C	1.3959220	1.6385430	4.7719190
H	1.2343460	2.0371810	5.7680990
C	2.6243490	1.8233310	4.1328440
H	3.4213200	2.3672660	4.6311970
C	6.0383870	6.5812190	-0.7962940
C	6.1550280	7.0226970	-2.1235040
C	5.9248180	8.3444580	-2.4914920
C	5.5570820	9.2756410	-1.5245580
C	5.4281190	8.8752920	-0.1978820
C	5.6736390	7.5508380	0.1504030
F	6.4795750	6.1577610	-3.0958890
F	6.0380770	8.7209040	-3.7714410
F	5.3284300	10.5462930	-1.8676900
F	5.0878410	9.7699620	0.7384850
F	5.5648270	7.2228790	1.4468190
C	8.8345860	-2.4765320	1.7848180
C	9.1318480	-3.4718610	0.8465100
C	9.7177060	-4.6823820	1.2029350
C	10.0324360	-4.9256270	2.5369170
C	9.7504200	-3.9600260	3.4989630
C	9.1658420	-2.7560760	3.1165310
F	8.8159600	-3.2884950	-0.4472150
F	9.9731040	-5.6132670	0.2754100
F	10.5965160	-6.0832400	2.8929260
F	10.0581730	-4.1868170	4.7822490
F	8.9294430	-1.8469810	4.0745190
O	2.1087540	0.1599070	0.9428770
C	1.0688520	-0.4158090	0.1573960
H	0.2256140	0.2760200	0.0501710
H	0.7047580	-1.3585790	0.5831270
C	1.5910960	-0.7346550	-1.2372340
O	0.8102990	-1.0643870	-2.1250300
N	2.9427780	-0.6649990	-1.3958120
C	3.5686390	-0.8527440	-2.6971620

H	2.7968400	-0.6879180	-3.4534570
C	4.0715830	-2.2855460	-2.9444950
O	4.3410850	-2.6511970	-4.0960000
C	4.7203790	0.1397400	-2.9050940
H	5.4892550	0.0187580	-2.1342180
N	4.2329620	-3.0815020	-1.8657670
H	3.9094650	-2.7444580	-0.9683650
C	4.8592410	-4.4061670	-1.9371830
C	3.8249380	-5.5086450	-2.2806970
O	3.6548530	-6.4979450	-1.5721940
C	5.6016260	-4.7130950	-0.6424150
H	4.9227720	-4.6884040	0.2154390
H	6.4044610	-3.9889830	-0.4913470
H	6.0323770	-5.7145460	-0.6905210
N	3.1232880	-5.2665700	-3.4221280
H	3.4151070	-4.4693040	-3.9831380
C	2.1499370	-6.2026590	-3.9846830
C	2.7738770	-7.5311080	-4.4292690
C	0.9274540	-6.4423770	-3.0698560
O	0.1990020	-7.4204680	-3.2418290
N	0.6633880	-5.4819610	-2.1522410
H	1.3406190	-4.7514740	-1.9827870
C	-0.4361730	-5.6037350	-1.2003730
H	-1.3075340	-5.9711340	-1.7507590
C	-0.1097620	-6.5774840	-0.0572420
H	-0.9592800	-6.6670160	0.6275970
H	0.7574010	-6.2172830	0.5014310
H	5.1833620	-0.0324590	-3.8785680
H	4.3450340	1.1656720	-2.8694180
H	5.5645030	-4.3609920	-2.7750300
H	1.7418100	-5.6989570	-4.8690970
H	0.1129040	-7.5629910	-0.4703960
H	2.0025540	-8.1735990	-4.8561350
H	3.2250770	-8.0427530	-3.5773910
H	3.5440360	-7.3451420	-5.1826270
H	3.4694120	-0.2450280	-0.6395970
C	-0.6864280	-4.1975670	-0.6420690
N	-1.9335020	-3.7053080	-0.7969260
H	-2.5909740	-4.2225900	-1.3631790
O	0.2221190	-3.5853900	-0.0715120
N	-5.6647220	-0.5620030	0.0663860
N	-16.9709510	1.0372750	0.2778040
O	-5.7379820	-1.3528490	2.2077360
O	-5.6048780	0.1462010	-2.1046720
O	-17.0093610	0.2219460	2.4185110
O	-16.8591560	1.8333460	-1.8742580
C	-6.3479020	-0.9028400	1.2422650
C	-7.8118430	-0.6907200	1.2523990
C	-8.4794230	-0.1828300	0.1112350
C	-7.7388710	0.1225290	-1.0567490
C	-6.2745810	-0.0847300	-1.1027420
C	-8.3915950	0.6172390	-2.1737440
H	-7.8125130	0.8438130	-3.0617390
C	-9.7745530	0.8223150	-2.1552580
H	-10.2395540	1.2121590	-3.0517290
C	-10.5458540	0.5369050	-1.0265440
C	-9.8941380	0.0178310	0.1373930
C	-10.6220240	-0.3057460	1.3266250
C	-9.9208610	-0.8040440	2.4268450
C	-8.5362590	-0.9949860	2.3930740
H	-8.0123370	-1.3834070	3.2590020
C	-12.0781020	-0.1044010	1.3514510
C	-12.8545580	-0.4097110	2.4712780
H	-12.3934060	-0.8133910	3.3637050
C	-14.2390650	-0.2108460	2.4858000
H	-14.8221220	-0.4560140	3.3660380

C	-14.8870510	0.3036640	1.3753030
C	-14.1410100	0.6262580	0.2180710
C	-12.7272480	0.4228710	0.1908310
C	-11.9999630	0.7519610	-0.9961430
C	-12.7007290	1.2679770	-2.0883420
C	-14.0847270	1.4669660	-2.0499380
H	-14.6071080	1.8698680	-2.9099100
C	-14.8091420	1.1518150	-0.9121680
C	-16.2745270	1.3734820	-0.8979380
C	-16.3558470	0.5066770	1.4190950
C	-4.2053590	-0.7574740	0.0468790
H	-3.8468530	-0.5692350	1.0593240
C	-3.8138730	-2.1689190	-0.4041900
H	-4.1913780	-2.3356220	-1.4199680
H	-4.2874210	-2.9033070	0.2560520
C	-18.4508690	1.2664390	0.2821260
H	-18.6391300	1.6809690	-0.7072570
C	-18.8604330	2.3164360	1.3208120
H	-18.2859830	3.2383020	1.1872680
H	-18.7165820	1.9550880	2.3397110
C	-19.2285230	-0.0490290	0.3993870
H	-19.0957850	-0.5119870	1.3780310
H	-18.9115900	-0.7565990	-0.3729730
H	-10.4434780	-1.0555770	3.3408830
H	-12.1785040	1.5294180	-2.9999220
C	-2.2973300	-2.3553760	-0.3744120
H	-19.9190700	2.5579200	1.1823320
H	-20.2939880	0.1537110	0.2512440
H	-3.7925130	-0.0099960	-0.6308410
H	-1.9133600	-2.2050690	0.6401720
H	-1.7967880	-1.6228250	-1.0206990
H	6.8205540	0.9779780	0.9654260

Turn1,4-Cor-(Ala)$_4$-PDI$_{opt}$ in toluene

Energy total = -5475.31209905 a.u.

Symbol	X	Y	Z
C	8.8389990	3.0964490	-1.0684730
C	9.4646140	4.3191290	-1.4209600
H	10.5110770	4.4424170	-1.6614560
C	8.5129850	5.3330800	-1.3177890
H	8.6838070	6.3902420	-1.4625760
C	7.2819260	4.7509330	-0.8977120
C	6.0338040	5.2844650	-0.4782160
C	5.1095250	4.5282940	0.2711210
C	3.7332880	4.7883530	0.5352940
H	3.1876380	5.6395450	0.1542110
C	3.2163280	3.7517860	1.2800510
H	2.1924680	3.6384730	1.6040860
C	4.2462730	2.7908120	1.5177330
C	4.1411140	1.5616180	2.1891920
C	5.1067700	0.5256130	2.2319120
C	5.0225270	-0.7058460	2.9624310
H	4.2002230	-0.9772590	3.6074830
C	6.1561130	-1.4476120	2.7099640
H	6.3919420	-2.4225640	3.1109390
C	6.9827620	-0.7015280	1.8159750
C	8.2457060	-0.9955770	1.2497790
C	8.8978940	-0.1085160	0.3618800
C	10.2606380	-0.1409080	-0.1401900
H	10.9805780	-0.9333260	0.0133020
C	10.4666090	1.0441370	-0.8012320
H	11.3721470	1.3752620	-1.2919020
C	9.2268450	1.7757270	-0.7071020
N	7.5298940	3.4075370	-0.8160610

H	6.8389020	2.6911890	-0.6675730
N	5.3811600	3.2850350	0.8679720
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O	3.8102060	-6.5952600	-1.4441290
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C	-3.7183150	-2.3825130	-0.3100780
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H	-18.0995540	3.3703090	0.9665510
H	-18.5417270	2.1839480	2.2147450
C	-19.1321810	0.0603420	0.4273890

H	-19.0031310	-0.3331310	1.4363160
H	-18.8413920	-0.7096930	-0.2938390
H	-10.3569450	-0.9956300	3.3724250
H	-12.0612330	1.2469100	-3.1052300
C	-2.2014650	-2.5601170	-0.2528660
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H	-3.6985710	-0.2384660	-0.6391190
H	-1.8345880	-2.3761940	0.7624680
H	-1.6934860	-1.8468080	-0.9147500
H	6.7471370	1.1029500	0.8771160

$(Ala)_4$-PDI_{opt} in toluene

Energy total = -2517.08514256 a.u.

Symbol	X	Y	Z
C	-5.3149520	-0.7097470	-3.2894470
H	-4.3580210	-0.2002610	-3.4156820
C	-5.3294200	-1.6552230	-2.1066720
O	-6.3613560	-2.2367390	-1.7431500
N	-4.1419930	-1.8549070	-1.4804960
H	-3.3567030	-1.2470900	-1.6977610
C	-4.0545390	-2.7308160	-0.3176500
H	-4.4535950	-3.7108010	-0.6028910
C	-2.5972420	-2.8716680	0.1261160
H	-2.2039470	-1.9032570	0.4462450
H	-2.5210020	-3.5668260	0.9662720
H	-1.9844870	-3.2540860	-0.6948310
C	-4.9028410	-2.1478970	0.8312560
O	-4.6990310	-1.0055910	1.2516270
N	-5.8678790	-2.9525550	1.3343500
H	-6.0512020	-3.8249700	0.8605290
C	-6.8118600	-2.5058430	2.3662900
C	-7.5811260	-1.2175500	1.9552870
O	-7.9673290	-0.4311970	2.8147420
C	-6.1525830	-2.3465390	3.7375050
H	-5.3659620	-1.5915650	3.6963180
H	-5.7210520	-3.2989730	4.0572910
H	-6.8989680	-2.0261420	4.4653140
N	-7.8391900	-1.1017270	0.6253310
H	-7.3810710	-1.7441120	-0.0142240
C	-8.5599770	-0.0046380	-0.0221890
C	-9.8911420	0.3603050	0.6467580
C	-7.7176840	1.2618620	-0.3057850
O	-8.2304760	2.1983050	-0.9227490
H	-7.5700310	-3.2951710	2.4289350
H	-8.7864610	-0.3800270	-1.0268100
H	-10.3755520	1.1361630	0.0514530
H	-9.7323990	0.7256120	1.6608780
H	-10.5422580	-0.5176070	0.6883240
N	-6.4186690	1.2544650	0.0671310
H	-6.0327590	0.4742980	0.5875720
N	-1.7104880	2.2368460	-0.8830820
N	9.2340560	-0.7606490	0.4315380
O	-2.0890180	0.3155890	-2.0584420
O	-1.3511640	4.0932960	0.4046000
O	8.8455440	-2.5989010	-0.8807640
O	9.5436050	1.0987730	1.7453970
C	-1.2939380	1.0322440	-1.4424780
C	0.1275510	0.6620280	-1.2779240
C	1.0046010	1.4770050	-0.5208480
C	0.5153460	2.6629460	0.0765020
C	-0.8945900	3.0744000	-0.0972580
C	1.3675790	3.4559560	0.8272330
H	0.9775180	4.3615310	1.2779730

C	2.7070420	3.0939960	0.9975530
H	3.3344230	3.7452490	1.5928480
C	3.2362240	1.9363620	0.4225940
C	2.3743450	1.1032350	-0.3597830
C	2.8487560	-0.0928820	-0.9867730
C	1.9489160	-0.8619190	-1.7285430
C	0.6077510	-0.4945710	-1.8708830
H	-0.0721660	-1.1071910	-2.4519310
C	4.2610300	-0.4702980	-0.8313290
C	4.7988290	-1.6129720	-1.4272330
H	4.1762910	-2.2578920	-2.0346460
C	6.1431110	-1.9665190	-1.2681700
H	6.5403580	-2.8586100	-1.7387500
C	6.9895350	-1.1815580	-0.5039230
C	6.4893960	-0.0132330	0.1160600
C	5.1191830	0.3583210	-0.0420500
C	4.6437660	1.5482640	0.5934450
C	5.5389090	2.3021430	1.3552010
C	6.8783670	1.9278100	1.5063820
H	7.5564310	2.5278080	2.1023000
C	7.3606230	0.7829010	0.8949460
C	8.7858530	0.4110400	1.0699980
C	8.4106120	-1.5834520	-0.3475850
C	-3.1187010	2.6382620	-1.0761420
H	-3.3883570	2.3695870	-2.0990060
C	-4.0588380	1.9490140	-0.0834880
H	-3.7648350	2.2040190	0.9400230
H	-3.9479410	0.8676690	-0.1864670
C	10.6736160	-1.1293920	0.6193210
H	11.0542910	-0.3241410	1.2463010
C	11.4446320	-1.1057170	-0.7049310
H	11.3145730	-0.1451730	-1.2130160
H	11.1245670	-1.9057110	-1.3734120
C	10.8234700	-2.4447000	1.3916520
H	10.4670920	-3.2963790	0.8109740
H	10.2736310	-2.4044520	2.3370400
H	2.2780810	-1.7720460	-2.2137090
H	5.2083820	3.2055660	1.8519540
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H	12.5117640	-1.2315470	-0.4958690
H	11.8812100	-2.6009080	1.6262880
H	-3.1505020	3.7221310	-0.9688990
H	-5.6975880	2.5358290	-1.3983290
H	-5.7804630	3.2616030	0.1947700
H	-5.5449470	-1.2773790	-4.1962230
H	-6.1087040	0.0297310	-3.1572330

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